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TECHNICAL ABSTRACTS

DETERMINATION OF GLOBAL REACTION RATE DURING LASER INDUCED DECOMPOSITION AT STATIC HIGH PRESSURES

T.P. Russell and G.I. Pangilinan, Chemistry Division, Naval Research Laboratory, (Presented at the *1998 March Meeting of the American Physical Society*, Held in Los Angeles CA, March 1998).

The laser induced decomposition of hexahydro-1,3,5-trinitro-1,3,5 triazine ($C_3H_6N_6O_6$,RDX), trinitro azetidine ($C_3H_4N_3O_6$, TNAZ) and ammonium perchlorate (NH_4ClO_4 ,AP) at static high pressure in the range of 0.6-2.0 GPa is presented. The samples are loaded in a gem anvil cell and the reaction is induced with a single laser pulse (514 nm, 6 µs duration, 3-22 J/cm^2). The dynamic chemical processes are probed using time resolved ultraviolet/visible absorption spectroscopy, during and up to 20 µs after the laser pulse. In all three materials, decomposition is characterized by a time-dependent increase in absorbance from 300-500 nm. This absorption change is directly proportional to the mole fraction of reaction and provides a measurement of the global reaction rate. The reaction rate is determined to be dependent on the sample, the initial pressure, and the laser fluence. The chemical decomposition is modeled using a three term reaction rate equation encompassing initiation, growth, and coalescence. A description of the differences in the decomposition kinetics for each material will be provided. Finally, the implications of these measurements to models of macroscopic energy release rates will be addressed.

CHARACTERIZATION OF RAMAN SPECTRAL CHANGES IN ENERGETIC MATERIALS AND PROPELLANTS DURING HEATING

N.F. Fell Jr, J.A. Vanderhoff, R.A. Pesce-Rodriguez and K.L. McNesby, Weapons and Materials Research Directorate, Army Research Laboratory, Aberdeen Proving Ground, MD 21005 (Army Research Laboratory Final Report ARL-TR-1743, 32 pp., August 1998).

Raman spectroscopy has been shown to be a useful tool for characterizing neat crystalline explosive samples and for identifying principle components in many propellant and explosive formulations. Herein, we report recent measurements of Raman spectra of explosives and propellant formulations during bulk heating and recent measurements of laser heating of the samples during measurement of Raman spectra. The results of these measurements are important to investigators using Raman spectroscopy to measure vibrational spectra of burning propellant samples.

CHARACTERIZATION OF TURBULENT FLAMES BY RAMAN, RAYLEIGH AND LIF LASER TECHNIQUES
W. Meier, O. Keck, V. Bergmann, D. Wolff, V. Jorres and W. Stricker, Institut fur Physikalische Chemie der Verbrennung, DLR Stuttgart, Pfaffenwaldring 38, D-70569 Stuttgart (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

Two different types of nonpremixed turbulent flames were investigated by single-pulse laser techniques: (1) A jet diffusion flame (Re=15200) fueled by a mixture of CH_4, H_2, and N_2 and (2) a confined swirling natural gas/air flame (Re=42900). The main goals of the investigations have been the development and study of various quantitative and qualitative laser techniques and the measurement of comprehensive data sets which yield a detailed characterization of these flames and which can be used for the validation of mathematical flame models.

A flashlamp pumped dye laser (489 nm, 2μs pulse duration, 2 J pulse energy) was used for the excitation of spontaneous Raman and Rayleigh scattering. From the Raman signals, the PDFs of the major species concentrations (CH_4, H_2, O_2, N_2, H_2O, CO_2, CO) have been determined in quantitative pointwise measurements with a spatial resolution of 0.6 mm. The temperature was deduced from the total number density and, in addition, from the Rayleigh scattering signals using the actual Rayleigh cross section determined from the Raman data. The radial profiles of the mean values and rms fluctuations which have been derived from the PDFs yield a general characterization of the flames and the correlations between various quantities give an insight into more subtle processes of the turbulence-chemistry interaction. Effects of differential diffusion and flame stretch have been identified and will be discussed in the poster.

In addition to the point measurements, two-dimensional distributions of OH, CH, NO and temperature have been measured in order to visualize the structures within the flames. For these measurements, the output of a Nd:YAG pumped optical parametric oscillator was formed to a light sheet and irradiated vertically into the flame. The laser induced fluorescence and Rayleigh scattering were detected by an intensified CCD camera. The LIF signals of OH and CH, which served as an indicator for the size and shape of the reaction zones, revealed that the turbulent flowfield of the jet flame was laminarized in the flame zone in the near-nozzle region. Further downstream, the OH distributions became broad and diffuse, whereas the CH distributions remained thin, indicating that the reactions take place in the thin flamelet-like layers throughout the flame. The 2-D images of LIF from NO reflected the structures of the flowfield and showed an increasing NO level with growing downstream position caused by accumulation of NO in the exhaust gas. The 2-D Rayleigh scattering signals were converted into quantitative temperature distributions reflecting, for example, temperature gradients, thermal dissipation rates, and the occurrence of local flame extinction.

The poster will discuss various aspects of the measuring techniques and the characteristics of the flames investigated. Model calculations for these flames are currently in progress by several research groups and we hope to present some comparisons between experimental and theoretical results.

MILLIMETER-WAVE TIME RESOLVED STUDIES OF THE FORMATION AND DECAY OF CO^+
L. Oesterling, E. Herbst and F. De Lucia, Ohio State University (Presented at the *1998 Joint Meeting of the American Physical Society and the American Association of Physics Teachers*, Held in Columbus OH, April 1998).

Since the rate constants for ion-molecule interactions are typically much larger than neutral-neutral interactions, understanding ion-molecule interactions is essential to interpreting radio astronomical spectra from interstellar clouds and modeling the processes which lead to the formation of stars in these regions. We have developed a cell which allows us to study ion-molecule interactions in gases at low temperatures and pressures by using an electron gun technique to create ions. By centering our millimeter-wave source on a rotational resonance and gating the electron beam on and off, we are able to study the time-dependent rotational state distribution of the ion during its formation and decay, and so learn about excitation and relaxation processes as functions of temperature, pressure, electron beam energy, and electron beam current.

PHOTOIONIZATION CROSS SECTION OF THE $6P_{3/2}$ STATE OF CESIUM

B.M. Patterson, T. Takekoshi and R.J. Knize, U.S. Air Force Academy (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

We report measurements of the photoionization cross section for the $6P_{3/2}$ state of cesium. Cross sections were determined for a range of wavelengths by measuring the photoionization rate of cesium atoms confined in a magneto-optical trap. The photoionization rate was determined by monitoring the decay of trap fluorescence after exposure to ionizing laser radiation. One series of measurements was made using an Ar ion laser for discrete wavelengths between 458 and 502 nm. Preliminary results at 488 nm indicate a cross section of $1.3\text{x}10^{-17}$ cm^2. Additional measurements are being carried out over a continuous wavelength range of 400 to 500 nm using a mode-locked fs Ti:Saphire laser.

CHEMI-IONIZATION OF EXCITED MERCURY

R.L. Martin, J.S. Cohen and L.A. Collins, Los Alamos National Laboratory (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

We report calculations of the chemi-ionization cross sections for the collisions of Mercury (Hg) atoms in the excited ^3P and ^1P states, examining both the Penning and Associative Ionization mechanisms. The $Hg_2{}^{**}$ system presents an intricate situation for chemi-ionization. Chemi-ionization is not energetically possible when only one of the atoms is excited. Some of the asymptotes correlating to two excited (^3P) atoms still lie just below the Hg^+ energy, so only associative ionization is possible, while others lie just above it, enabling both associative and Penning ionization. Potential energy curves for the excited neutral and the ion molecular states are generated using relativistic core potentials and full configuration interaction involving the active electrons. The influence of core-valence correlation and the errors associated with the interaction curves will be discussed. We will present cross sections for both Penning and associative ionization.

QUANTITATIVE MODEL FOR SPIN-POLARIZED PENNING IONIZATION OF O_2

G.H. Rutherford, Department of Physics, Illinois State University (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

Penning ionization in gas phase collisions between $He(2^3S)$ metastable atoms and simple molecules has in recent years been aided by electron spin labeling, in which the He electrons are spin-polarized via optical pumping and energy-resolved spin polarization measurements are made on the ejected electrons. Such data for O_2 show the effects of depolarizing mechanisms in that the ejected electron polarization is only about one-third that of the metastable atoms, and clear structure in the energy-resolved polarization data is seen. We present a quantitative model for these data that uses angular momentum coupling and an assumed shape for each product ion state's contribution to the electron energy distribution. The effect of the transition to a strongly attractive ion-pair entrance potential is described. It appears that spin-orbit coupling in the collision complex prior to ionization is negligible.

PHOSPHOROUS COMPOUNDS AS FLAME INHIBITORS: ANALYSIS OF IONIC INTERMEDIATES

P. Hebgen and K.-H. Homann, Institut fur Physikalische Chemie, Technische Universitat Darmstadt, Petersenstr. 20, D-64287 Darmstadt, Germany (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

A current issue is to find substitutes for the generally used halogen-containing flame suppressants because of their ozone depleting qualities. Phosphorous compounds are also know to be effective flame inhibitors.

Analysis of the intermediates that are formed in phosphorus-doped flames is necessary for the understanding of the inhibition mechanisms. The large electron affinities of the phosphorus oxides and related compounds offer a good chance to detect the intermediate species in the inhibiting mechanism and the products from reactions with flame radicals in the form of their respective ions.

Negative and positive flame ions from a premixed low pressure (27 mbar) ethyne/oxygen flame doped with 0.1 mol-%) of trimethyl phosphate or tris(dimethylamino)phosphine were analyzed with a reflectron time-of-flight mass spectrometer in the mass range up to 400 u. The velocity of the unburned gas was 42 cm/s and the C/O ratio was varied in the range from 0.4 to 1.0(ϕ=1 to 2.5).

Most of the negative ions are the anions of polyphosphoric acids, which are ionized by scavenging electrons from the flame. The ions with the highest concentrations correspond to the molecular formulas PO_3^-(79 u), $HP_2O_6^-$(159 u), and $H_2P_3O_9^-$(239 u), while PO_2^-(63 u), $P_3O_8^-$ (221 u), and $H_2P_4O_{11}^-$(301 u) are less abundant by more than a factor of 10. The ions could be divided into different groups depending on their structure. With the knowledge of the structure, a P/H/O matrix could be set up, wherein the ions appear as a band. The structure of the positive ions follows a rather complicated system of different principles.

The results obtained from the flame ions show that the doping substances originally decompose at their P-O and P-N bonds, respectively, the fragments reacting with the flame radicals. This can clearly be seen from the negative flame ions, where the high affinity of phosphorus to oxygen-containing radicals, O and OH, is demonstrated.

The investigation of the positive flame ions supports this observation. Besides the reactions with oxygen-containing radicals, there were ions that indicated also reactions with hydrocarbon radicals and H-atoms.

In the case of tris(dimethylamino)phosphine, the $N(CH_3)_2$-groups support the inhibition in two ways. On the one hand, the P-N bond decomposes easily, whereby the inhibitory effect of the phosphorus is increased. On the other hand, the resulting nitrogen containing radicals can also scavenge radicals and inhibit the flame.

The high concentrations of the product species from the inhibiting reactions at low distances from the burner show that the doping substances decompose already at low temperatures, that is, at the beginning of the combustion process. By that, radicals like H, O, and OH which promote the combustion processes are taken away. This causes a slow-down of the combustion.

EXPERIMENTAL EVALUATION OF CORONA DISCHARGE REACTOR FOR REMOVAL OF NO_x AND SMOKE IN DIESEL EXHAUST

T. Morimune, Shonan Institute of Technology, 1-1, Tsujidoh Nishikaigan, Fujisawa, Japan (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

In order to remove the NO_x and smoke contained in diesel exhaust gas, the gas is excited by passing through a corona discharge reactor in a high electric voltage field. An electrostatic smoke collector (ESC) is designed to collect diesel smoke particles electrically on a central electrode and smoke will be removed by a controlled burning (regeneration) process every 20 minutes. In a corona discharge reactor for NO_x removal (DRNR), the NO is oxidized to NO_2 , and

OH radical generated from H_2O in the gas reacts with the NO_2. NO_x concentration decreases as a result of formation of HNO_3. The ESC contains a 54 mm diameter tube with a 6 mm diameter roll of nichrome wire serving as a central electrode. The NO_x removal reactor has a copper wire electrode of 1.6 mm diameter. The discharge instability of ESC by the smoke accumulation on the electrodes is investigated, and a smoke removal rate, >90%, is obtained during 20 minutes under the condition of 16 kV, 2mA. As for DRNR, the effects of H_2O content in the exhaust gas and inlet temperature on the NO_x reduction are discussed. The NO_x removal rate, >80%, is obtained under the input power of 90 W (30 kV, 3 mA) and a gas flow rate of 15 liters/min.

Laser Induced Incandescence Measurements of Soot Concentration and Particle Size

J.H. Frank, K.R. McManus, M.G. Allen and W.T. Rawlins, Physical Sciences Inc., 20 New England Business Center, Andover, MA 01810 (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

There exists an increasing need for nonintrusive measurements of soot number density and particle size in practical combustion devices. An optical probe for the detection of soot particles in gas turbine combustors and exhausts is currently under development. The probe is based on the technique of laser induced incandescence (LII), in which soot particles are rapidly heated by a pulsed laser, and the resulting thermal radiation from the particles is detected. The LII signal is proportional to the initial soot concentration. This proportionality depends on several factors, including the laser energy absorbed by the particles, heat and mass loss from the particles by vaporization, and conductive heat loss from the particles to the surrounding gas. Each of these factors is dependent on particle size, and together they govern the initial heating rate, maximum temperature and cooling rate of the particles.

In developing an LII-based probe, we have conducted a detailed investigation of the LII technique. Experiments were performed in premixed and nonpremixed ethylene/air flames. Laser extinction measurements above a premixed flat flame were used to calibrate the LII signal for determining soot concentrations. To test the sensitivity of the LII technique, the soot concentration in the flat flame was varied by changing the equivalence ratio. The results demonstrated the feasibility of LII measurements of soot concentration spanning five orders of magnitude. Particle size measurements were performed by determining the soot temperature and the particle cooling rates from the LII signal. This required a detailed study of the spectral and temporal characteristics of the LII emission. We conducted such a study in a coannular laminar nonpremixed flame, for which the soot characteristics have been extensively documented in the literature. A gated spectrometer was used to record the spectrum of the LII signal during a 30 ns period with varying time delays relative to the laser pulse. The resulting spectra showed good agreement with blackbody radiation spectra that were corrected for variations in soot emissivity. These results indicated that the soot temperature and cooling rates could be accurately measured with a high-speed pyrometer. Subsequently, a fast-response two-color pyrometer was used to measure the particle temperatures as a function of time. Particle sizes were determined by comparing the measured soot temperatures and cooling rates with those predicted by a model of the conductive cooling process. Measurements of particle vaporization rates differed significantly from predictions of an equilibrium vaporization model.

The results indicate the LII can provide nonintrusive measurements of soot concentrations at low levels relevant to exhaust emissions of gas turbine engines. Implications for particle sizing measurements with LII will be discussed.

On Soot Yield and Soot Mass Formation in the Pyrolysis of Acetylene/Benzene Mixtures

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In the pyrolysis of C_2H_2 and C_6H_6, the variation of the mixture ratio of the these hydrocarbons on the soot yield and the soot mass growth rates was studied. The experimentally determined soot mass growth rates were compared with computed formation rates of high molecular polyaromatic hydrocarbons (PAH). The total carbon content of the mixtures was maintained at a constant value of 6 mol/m^3. The temperature in the determined pyrolysis was 2000 K, and the pressure 6.0 MPa.

The experiments were carried out behind reflected shock waves in a 70 mm inner diameter steel shock tube consisting of a 4.5 m driven section and a 3.5 m driver section. Piezo-electric pressure conductors were used to measure the shock speed and the pressure time profile. Shock parameters were computed on the base of the standard procedure using the measured incident shock speed. The conversion of hydrocarbon to soot was determined by the attenuation of the light beam from a 15 mW He-Ne laser at 632.8 nm. The extinction profiles I(t) were converted into soot yield profiles SY(t) using Beer's law, a refractive index of m=1.57-0.56i, a soot density of 1.86 g/cm^3 and the molar mass of carbon. The test gas mixtures were prepared manometrically and mixed by convection. The gases C_2H_2(>99.6%), and Ar(>99.9%) were used without further purification. Benzene (>99.9%) was purified by distillation.

The formation rates of high molecular PAH were computed taking the combinative ring-ring condensation of aromatics into account. In the experiments, it was found that the soot yield as well as the soot mass growth rates strongly depend on the mixture ratio of C_2H_2/C_6H_6 in the pyrolysis gases. The drastic decrease of the soot mass growth rates with increasing C_2H_2 content of the mixtures is in line with the computed decline of the formation rate of high molecular PAH.

Growth of Nano-Particles in an Acetylene Radiofrequency Discharge

G. Chandhoke, C. Eggs and U. Kortshagen, University of Minnesota, Mechanical Engineering, 111 Church Street SE, Minneapolis, MN 55455 (Presented at the *51st Annual Gaseous Electronics Conference and the 4th International Conference on Reactive Plasmas*, Held in Maui HI, October 1998).

The growth mechanism of nano-sized carbon particles has been investigated. Particles were grown in a capacitively coupled radiofrequency discharge. Pure acetylene (C_2H_2) as well as argon diluted acetylene have been used as feed gases at different flow rates, pressures and discharge powers. Growth behavior of particles was studied by transmission electron microscopy (TEM) measurements after different plasma-on times t_{on}($1s<t_{on}<60s$). For $t_{on}>10$ s these measurements clearly show two different size groups of particles. The average size of the smaller particles remains constant at approximately 30 nm whereas larger particles of the second group continue to grow. The particle surface grows at a constant rate and for $t_{on}=60$ s the particle diameter is approximately 350 nm (at $P_{discharge}=50$ W, 100 mtorr). The elemental composition of the particles was determined by X-ray photoelectron spectroscopy. From the infrared spectra of the particles the hydrogen content and the amount of double and triple C bonds was estimated and compared to the feed gas C_2H_2.

EFFECTS OF GAS FLOW ON PARTICLE GROWTH IN SILANE RADIOFREQUENCY DISCHARGES
Y. Matsuoka, M. Shiratani, T. Fukuzawa and Y. Watanabe, Kyushu University, Japan, and K. Kim, Kangwon National University, Korea (Presented at the *51st Annual Gaseous Electronics Conference and the 4th International Conference on Reactive Plasmas*, Held in Maui HI, October 1998).

Effects of gas flow on particle growth in silane radiofrequency discharges are studied mainly using a polarization-sensitive laser light-scattering method. Gas of He+SiH_4 (5%) is supplied from the radiofrequency shower electrode and exhausted from the grounded mesh electrode. For 80 Pa and radiofrequency power (6.5 MHz) of 80 W, particle growth rate increases to a maximum value of 40 nm/s when increasing the gas flow rate from 2 to 10 sccm, then the rate decreases considerably with further increasing the flow rate to 30 sccm. The former increase is mainly attributed to the increase in supply of short-lifetime radicals contributing to the rapid particle growth. The latter decrease suggests that neutral clusters, a diffusion time of which is longer than a gas residence time in the particle growth region, play a significant role in particle growth. For all the flow rates, particles begin to be observed around plasma/sheath boundary near the radiofrequency electrode and some of them flow to the grounded electrode after they grow above 100 nm and then trapped around plasma/sheath boundary there. Moreover some particles above 120 nm flow through the grounded mesh electrode into the downstream region at a certain time in the discharging period. This result implies that some large particles may deposit on the film surface in CVD reactors having shower radiofrequency electrode.

CHARACTERIZATION OF PARTICLE GROWTH IN A SILANE PLASMA
M.A. Childs, A. Gallagher, JILA, NIST and University of Colorado at Boulder (Presented at the *51st Annual Gaseous Electronics Conference and the 4th International Conference on Reactive Plasmas*, Held in Maui HI, October 1998).

Particles grow in silane plasmas used to make amorphous silicon films, and some particles escape the plasma and become incorporated in the film. We report measurements of particle size and density as a function of discharge parameters in the initial states of a radiofrequency, parallel plate discharge. When the particles are large enough to be observable (radius $R>4$ nm), the particles usually grow linearly in time at a rate consistent with growth by SiH_3. The data indicate that more rapid growth occurred for $R<2$ nm; possible causes for this will be presented. An exception to linear growth for $R>4$ nm occurs at higher pressures and radiofrequency voltages: the growth rate increases after an induction period, perhaps due to Si_mH_j with $m>1$.

ATOMIC SPECTRA DATABASE
D.E. Kelleher, W.C. Martin, W.L. Wiese, A. Musgrove, J.R. Fuhr, J. Sugar, J. Reader, K.J. Olsen, P.J. Mohr and G.R. Dalton, National Institute of Standards and Technology (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

Our Atomic Spectra Database contains data for radiative transitions and energy levels in atoms and atomic ions. The URL is: http://physics.nist.gov/asd. Version 2.0, which will be put on-line this year, includes data for observed transitions of 99 elements and energy levels of 52 elements. It contains data on 950 spectra, with 70,000 energy levels and 90,000 lines from 0.1 nm to 200 µm, 40,000 of which have transition probabilities. All current NIST-evaluated data associated with each transition are combined under a single listing. Many options, search criteria, and a "Help" file are provided. Energy level data are included for most spectra of H-Kr(Z=1-36), Mo(Z=42), plus up to the first five spectra of the rare earth elements (Z=57-71). Classified lines with transition probabilities are included for most spectra of H-Ni(Z=1-28), including new extensive transition probability tables for C, N, and O, and selected transition probabilities are listed for the first two spectra of Cu-Es(Z=29-99). At a minimum, wavelengths with relative intensities are included for the prominent lines of up to the first five spectra of all elements, and comprehensive wavelength lists of classified lines with relative intensities are included for all spectra of Mg, Al, S, Sc, plus Be(I), O(II) and Ne(I).

A CLASS IV CHARGE MODEL FOR MOLECULAR EXCITED STATES

J. Li, B. Williams, C.J. Cramer and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *J. Chem. Phys.*).

We present a new parameterization for calculating class IV charges for molecules containing H, C, N, O, F, Si, P, S, Cl, Br, and I from wave functions calculated at the intermediate-neglect-of-differential-overlap-for-spectroscopy (INDO/S) level. First we readjust the oxygen parameters in INDO/S on the basis of electronic excitation energies; this yields a new set of parameters called INDO/S2. Then we parameterize the charge model. The new model, called Charge Model 2 for INDO/S2 (CM2/INDO/S2), is parameterized against the most accurate available data from both ab initio and experimental sources for dipole moments of ground and excited electronic states. For a training set containing 211 dipole moments of molecules in their ground states and 33 dipole moments of molecules in their first excited states, the CM2/INDO/S2 model leads to an RMS error in dipole moments of 0.26 D for ground states and 0.40 D for the excited states. The new model, INDO/S2 with CM2, systematically improves the $n \rightarrow \pi^*$ excitation energies and the dipole moments of the excited states of carbonyl compounds. We also parameterized a CM2 model for the standard INDO/S model (CM2/INDO/S), which predicts quite accurate dipole moments for ground states with an RMS error of 0.24 D.

STRUCTURE AND BONDING IN THE B^3P STATE OF CAr

K. Sohlberg, Oak Ridge National Laboratory, and D.R. Yarkony, The Johns Hopkins University (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

A spectroscopic study of the BAr van der Waals molecule [Yang and Dagdigian, *J. Chem. Phys.* 106, 6596 (1997)] revealed that the $C^2\Delta$ State has a remarkably large binding energy, $D_e \approx 3600\ cm^{-1}$. Associated theoretical work [Sohlberg and Yarkony, *J. Phys. Chem.* 101, 3166 (1997)] demonstrated that this surprisingly strong bonding can be described in terms of a new and unusual type of correlation-sensitive dative bonding. This unusual electronic structure is also reflected in a large external heavy atom effect (HAE) on the spin-orbit coupling of the $C^2\Delta$ and $1^4\Pi$ states. Similar but less pronounced bonding was demonstrated in BNe [Sohlberg and Yarkony, *J. Phys. Chem.* 101, 9520 (1997)]. These results inspired us to investigate the bonding in the $B^3\Pi$ state of CAr, as well as its spin-orbit coupling to the repulsive $^5\Sigma$ state. Preliminary results show that the CAr $B^3\Pi$ state is strongly bound and that its spin-orbit coupling to the $^5\Sigma$ state exhibits the HAE. The possible role of the new correlation-sensitive dative bonding and/or Rydberg orbital penetration effects will be addressed.

INITIAL AND FINAL STATE ANGULAR MOMENTUM ALIGNMENT IN THE ENERGY POOLING PROCESS: Ca(4s4p $^3P_1$+Ca(4s4p $^3P_1$)® Ca(4s4p $^1P_1$)+Ca(4s^2)

H.V. Parks and S.R. Leone, JILA and Department of Physics, University of Colorado, Boulder, CO 80309 (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

A detailed experimental study of the effects of initial Ca(4s4s $^3P_1$) state polarization and the resulting final Ca(4s4p $^1P_1$) state polarization in Calcium energy pooling is described. The initial state is aligned when it is excited from the ground state by a polarized laser pulse. Large periodic modulations in the energy pooling cross section are seen as the polarized initial states precess in an applied magnetic field. Seven of the eight parameters needed to completely describe the initial m-sublevel dependence of this j=1 plus j=1 collision process are obtained. The alignment of the final Ca(4s4p $^1P_1$) state is also studied. In addition, the coarse energy dependence of the polarization effects is deduced.

LIFETIME MEASUREMENTS OF CESIUM $5d^2D_{5/2,3/2}$ AND $11s^2S_{1/2}$ STATES USING PULSED LASER EXCITATION

D. Diberardino, C.E. Tanner, University of Notre Dame, and A. Sieradzan, Central Michigan University (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

We report measurements of the $5d^2D_{5/2}$, $5d^2D_{3/2}$ and $11s^2S_{1/2}$ state lifetimes in the ^{133}Cs atom to be 1281(9) ns, 909(15) ns, and 351(4) ns, respectively. A pulsed-dye laser selectively excites atomic Cs from the ground state via a single-photon quadrupole transition to the 5d states and via a two-photon electric dipole transition to the 11s state. A spectrometer-photomultiplier system detects the fluorescence from the decay of interest and a digitizing oscilloscope records the direct output of the photomultiplier. The data is fit to an exponential function to yield a value for the mean lifetime of the selected state.

SOLVENT INDUCED SPIN-ORBIT RELAXATION OF $I(^2P_{1/2})$ IN $I_2^-(CO_2)_n$ AND $I_2^-(OCS)_n$ CLUSTERS

A. Sanov, S. Nandi, T. Sanford and W.C. Lineberger, JILA, National Institute of Standards and Technology and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309 (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

Solvent induced spin-orbit relaxation of $I(^2P_{1/2})$ is studied following ultraviolet photodissociation of I_2^- within $I_2^-(CO_2)_n$ and $I_2^-(OCS)_n$ clusters. While ultraviolet dissociation of isolated I_2^- results in exclusive production of $I^-+I(^2P_{1/2})$, within a cluster interaction with the solvent induces nonadiabatic coupling of the $I^-+I(^2P_{1/2})$ and $I^-+I(^2P_{3/2})$ potentials and leads to dissociation on both $I(^2P_{1/2,3/2})$ spin-orbit asymptotes or I_2^- recombination. The production of $I(^2P)$ in both spin-orbit states, separated by 1 eV of energy, is manifest as a bimodal size distribution of 'uncaged' $I^-(CO_2)_k$ and $I^-(OCS)_k$ products. The nonadiabatic coupling occurs at long I-I^- range and is several times stronger in $I_2^-(CO_2)_n$, compared to $I_2^-(OCS)_n$ clusters. Evidence of different relaxation time scales in $I_2^-(CO_2)_n$ and $I_2^-(OCS)_n$ clusters is presented.

ELECTRONIC QUENCHING RATE CONSTANTS FOR Kr(5s[3/2]$_1$ and 5s¢ [1/2]$_0$) and Xe(6s[3/2]$_1$, 6s¢ [1/2]$_1$ AND SELECTED 6p, 6p¢ AND 7p) STATES BY VARIOUS REAGENTS AT 300 K

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Various laser based techniques, including pulsed one-photon excitation from the Xe(6s[3/2]$_2$) and Kr(5s[3/2]$_2$) metastable states, optical pumping from the metastable state, pulsed two-photon excitation from the ground state and pulsed two-photon amplified stimulated emission (ASE), have been used to selectively prepare a broad distribution of electronically excited states of Xe and Kr. Subsequent monitoring of the fluorescence from these states in the presence of added reagents permits two-body quenching rate constants to be measured. In many cases the products also have been identified, and state-to-state rate constants have been assigned. Examples of Kr* and Xe* excited states with different reagents will be selected to display various collisional properties of the Xe* and Kr* states, such as the role of the $Xe^+(^2P_{3/2})$ and $Xe^+(^2P_{1/2})$ ion-cores in intramultiplet relaxation processes and in reactive quenching with halogen containing molecules. The systematic increase in magnitude of quenching constants for a common reagent with increasing electronic energy of the Xe(6s,6s′,6p,6p′,7p) states will be presented. Two pairs of Xe(6p′,7p) states have a very large (~200 A^2) cross sections for intramultiplet transfer by collision with He and Ar; these large cross sections can be explained by a Demkov coupling mechanism. The majority of the presentation will be a description of the time-resolved two-photon ASE experiments, which provide a pulsed laboratory source of the $Xe(6s[3/2]_1)$, $Xe(6s'[1/2]_1)$ and $Kr(5s[3/2]_1)$ resonance states. By monitoring their resonance fluorescence in the vacuum ultraviolet, the decay rates of these Kr* and Xe* resonance states can be observed in the presence of added reagent gas and the two-body quenching rate constants can be measured with excellent reliability. The two-body rate constants for the resonance states obtained from these experiments will be compared to those for the Xe and Kr metastable states, which have been available for about 20 years.

CHEMICAL GENERATION OF $NCl(a^1D)$ MOLECULES BY THE REACTION OF CHLORINE ATOMS WITH AZIDE RADICALS AND MEASUREMENTS OF QUENCHING RATE CONSTANTS OF $NCl(a^1D)$

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The first electronically excited state of NCl, the $a^1\Delta$ state with a lifetime of about 2 s and an energy of 1.15 eV, is a candidate for gas phase energy-storage applications. The NCl ($a^1\Delta$) molecule can be generated with a high efficiency by the reaction of Cl atoms with the azide radical, N_3, which is generated by the $F+HN_3$ reaction. The room temperature, gas phase experiments consist of adding F and Cl atoms together with HN_3 to a pre-reactor section of a flow reactor with typical initial concentrations of $[HN_3]=2.0\times10^{12}$, $[F]=2.5\times10^{12}$ and $[Cl]=2.0\times10^{12}$ molecules cm^{-3} in 1 torr of Ar carrier gas. The flow reactor is a 7.0 cm diameter Pyrex glass pipe of 150 cm length. The reactor walls were coated with halocarbon wax to prevent the loss of F and Cl atoms and NF(a) and NCl(a) molecules by reaction at the walls. The F- and Cl-atom reaction rates with HN_3 and N_3 are sufficiently fast that the HN_3 is converted to NF(a) and NCl(a) in the pre-reactor. The NF(a) and NCl(a) relative concentrations are monitored along the flow reactor by observing the (a-X) transitions at 874 and 1077 nm, respectively, with a cooled photomultiplier tube. Quenching reagents are added to the main reactor and the pseudo first-order decay rates of NF(a) and NCl(a) are observed and converted to bimolecular rate constants.

$O_2(b^1S_g^+)$, $O(^1D)$ AND $(O_2^+ + e)$ RECOMBINATION IN THE LOWER THERMOSPHERE

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Night sky spectra taken with the HIRES spectrometer at the Keck I telescope on Mauna Kea have revealed emissions from $O_2(b^1\Sigma_g^+)$ in vibrational levels up to $v'=15$. Previously only $v'=0$ was known in the nightglow. Emissions from $v'=1$ are unexpectedly strong, comparable to $v'=2$, and variable from scan to scan. $v'=1$ emissions are visible up to $J'=50$ (requiring a temperature of more than 500 K, such as in the thermosphere), while $v'=2$ emissions are restricted to $J'<25$ (consistent with a temperature of 200 K near the mesopause, where O+O recombination would peak). Considering that quenching of $v'=1$ is about ten times faster than $v'=2$, we infer that separate mechanisms are responsible for production of $v'=1$ and the other vibrational levels. The principal source of $v'=1$ appears to be $O_2^+ + e \rightarrow O(^1D)$, followed by $O(^1D)+O_2 \rightarrow O_2(b^1\Sigma_g^+)_{v'=1}$. At twilight, this process should have a maximum emission yield below 150 km, rising to about 250 km as the night progresses. Simultaneous observation of $O(^1D)$ and $O_2(b^1\Sigma_g^+)_{v'=0,1,2}$ should provide new information about kinetics in the thermosphere.

RELATIVE BAND OSCILLATOR STRENGTHS IN THE FOURTH POSITIVE SYSTEM OF CO

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An optical absorption experiment using synchrotron radiation as a continuum source was used to measure band oscillator strengths in the ($A^1\Pi$-$X^1\Sigma$) electronic spectrum of CO. When referenced to the well established (5,0) band oscillator strength, our relative values for the (7,0) to (11,0) bands are most consistent with the recent experiments of Chan et al. and the theoretical predictions of Kirby and Cooper. These results help to resolve a discrepancy among experimental determinations of the CO band strengths, so that analyses of interstellar CO based on absorption from (A-X) bands are no longer hindered by uncertainties in oscillator strength. A similar technique is being applied to higher lying transitions in the CO spectrum.

OSCILLATOR STRENGTHS OF FINE-STRUCTURE TRANSITIONS IN NEUTRAL SULFUR

S.S. Tayal, Clark Atlanta University (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

Oscillator strengths and transition probabilities of electric-dipole-allowed and intercombination transitions from fine-structure levels of the ground $3s^23p^4$ configuration to the levels belonging to configurations $3p^34s$, $3p^35s$, $3p^33d$ and $3p^34d$ of neutral sulfur are calculated using extensive configuration-interaction wave functions. The relativistic corrections have been included through the Breit-Pauli Hamiltonian. Small adjustments to the diagonal elements of Hamiltonian matrices have been made so that the energy splittings are close to the measured values. Our oscillator strengths and radiative lifetimes are compared with several available theoretical, empirical, and experimental results.

ATOMIC TRANSITION PROBABILITIES IN Ti

D.E. Nitz, Saint Olaf College, and M.E. Wickliffe and J.E. Lawler, University of Wisconsin-Madison (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

We report the measurement of branching fractions and atomic transition probabilities for 92 lines connected to high lying, even parity levels in neutral Ti. Branching fractions are determined from six high current hollow cathode emission spectra recorded using the Fourier transform spectrometer at the National Solar Observatory. The absolute scale for normalizing the branching fractions is established using radiative lifetimes from recently reported time-resolved laser induced fluorescence measurements. Most of our reported transition probabilities are accurate to better than ±10%.

ABSOLUTE LINE INTEGRATED DENSITIES OF CF, CF_2 AND CF_3 IN A GEC REFERENCE CELL

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Tunable diode laser absorption spectroscopy, in the region around 1250 cm^{-1}, was used to measure line integrated densities of CF, CF_2 and CF_3 in a GEC reference cell, modified for inductively coupled plasma operation. The addition of a quartz ring around the source region stabilized and confined the plasma, making the plasma chemistry more like that found in industrial etch tools. Two common etching gas chemistries, C_2F_6 and CHF_3 , and two wafer surfaces, bare silicon and blanket photoresist, were investigated across a range of power and pressure Substantial amounts of undissociated C_2F_6 were also found in the C_2F_6 plasma. The determination of the absolute density of CF led to a reexamination of the literature data on the value of the transition dipole moment for this radical. Our conclusion from this investigation is that recent large scale ab initio calculations currently provide the only reliable value of this parameter, which is required in any calculation of absolute CF densities.

ABSOLUTE CONCENTRATIONS OF CH RADICALS IN LOW PRESSURE METHANE/AIR FLAMES WITH CAVITY RING-DOWN SPECTROSCOPY

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Cavity ring-down laser absorption spectroscopy (CRDS) is used to determine the number density of CH radicals in low pressure, steady, laminar methane/air flames. The results compare well with earlier absolute CH radical concentration measurements made with laser induced fluorescence (LIF). The flames are supported on a standard McKenna, porous plug burner with a 6 cm flame diameter. CRDS signals are readily observed using the CH(A-X) transition near 430 nm. With the laser wavelength tuned off resonance the ring-down time of 30 μs is dominated by the mirror reflectivity; whereas, tuned to a Q branch transition the ring-down time in a fuel rich ($\Phi=1.27$) flame decreases to 10 μs at the peak of the CH structure in the flame. This corresponds to 18 ppm CH in this 30 torr flame which is in quite good agreement with our earlier quantitative LIF measurements.

The application of CRDS to flame measurements is discussed. Like any absorption measurement, variations in concentration and temperature along the line of sight path complicate the interpretation of CRDS measurements. The spatial resolution of CRDS is limited by the focal parameters of the ring-down cavity and the laser divergence. However, CRDS provides a quantitative determination of absorption from time resolved measurements, which eliminates the need for precise measurements of absolute intensity or the need for an intensity stabilized laser light source. The combination of spatially resolved LIF and CRDS provides an opportunity for precise spatially resolved quantitative measurements of trace quantities of chemical intermediate free radicals.

SIMULTANEOUS PLANAR IMAGING OF OH-LIPF AND SHADOWGRAPHS AND PLANAR IMAGING OF CH-LIF IN A TWO-DIMENSIONAL VALVELESS PULSE COMBUSTOR

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Using a novel optical system, simultaneous imaging of Schlieren photography and OH-LIPF (Laser Induced Predissociation Fluorescence) have been carried out to examine combustion processes and flame structure in a two-dimensional valveless pulse combustor. Planar CH-LIF imaging have also been made, in order to obtain information on the behavior of the flame front during a cycle of pulsation.

The pulse combustor of a forced-ventilated type consists of a combustion chamber of a volume of 125 cm^3 and a tailpipe of a length of 976 mm, which is followed by an automobile muffler. The fuel used is commercial grade gaseous propane. The combustor is operated under a set of conditions of a fuel flow rate of $Q_{fN}=4.0$ l/min, an air flow rate of $Q_{aN}=103.5$ l/min, an overall equivalence ratio of $\phi=0.92$ and a pulsation frequency of $f_0=137.5$ Hz. Four quartz glass windows are employed for planar optical access.

In order to get simultaneous detection of OH-LIPF and shadowgraph images, two types of optical systems are combined with a beam-splitter (an uncoated quartz glass plate of 4 mm thickness), which is placed on the axis of the Schlieren optical system at 45°, so that the planar images of

OH-LIPF can be acquired simultaneously with the Schlieren images in the same direction. A tunable excimer laser (LPX150t; Lambda Physic) tuned to a wavelength of 248.5 nm is used for the planar OH-LIPF imaging. To detect the LIPF image at a wavelength of 308 nm due to (3,0) band of the ($A^2\Sigma$-$X^2\Pi$) system, employed is an image-intensified CCD camera (Streak Star II; La Vision) with a UV-lens (UV-Nikkor, 105 mm, F4.5) and an optical filter (center wavelength 330 nm, FWHM 85 nm) equipped. The Schlieren optical system used is composed of a Z-configuration concave mirror system and a flash (20 μs) Xenon lamp.

In the case of CH-LIF imaging, the excimer-laser-pumped dye laser which is tuned to a wavelength of 387 nm is used. The fluorescence at a wavelength of 431.5 nm due to (0,0) band of the ($B^2\Sigma$-$X^2\Pi$) system is detected with an optical filter (center wavelength 432.6 nm, FWHM 10.3 nm) and the CCD camera system above mentioned.

The results obtained in this investigation are summarized as follows.

(1) According to the simultaneous imaging of OH-LIPF and shadowgraphs and the planar imaging of CH-LIF, it is found that combustion takes place along the boundaries of a pair of large scale eddies of inflowing fresh mixture, but not within the entire eddy regions, exhibiting a pair of earlobe-shaped flame contours.

(2) It is also found that OH-radicals never disappear in the combustion chamber during the period of pulsation, although reacting flame front does not exist until the next fresh charge. This shows that the intermittent ignition is considered to be due to the combined effects of the thermal and chain-reaction processes in the residual hot combustion products in the last cycle.

These results point out an important concept which should be taken into account for designing a new devised pulse combustion system.

TWO-PHOTON ABSORPTION LASER INDUCED FLUORESCENCE OF ATOMIC NITROGEN BY AN ALTERNATIVE EXCITATION SCHEME

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A new two-photon absorption laser induced fluorescence (TALIF) scheme to monitor the ground state atomic nitrogen produced in a gas discharge is characterized. Excitation at 207 nm to the $(3p)^4S^o_{3/2}$ upper state is demonstrated to be superior to the traditional 211 nm excitation to $(3p)^4D^o_{7/2}$. Most striking is the low quenching rate of the upper $(3p)^4S^o_{3/2}$ state by N_2 at $k_q=6.7\times10^{-11}$ cm^3/s, nearly an order of magnitude lower than the traditional technique. The two-photon excitation rate at 207 nm is also measured to be a factor of 3 greater than the traditional scheme. The advantage in signal strength of the new TALIF scheme is shown to be especially pronounced at N_2 pressures above 1 torr. The TALIF technique is also compared to the indirect technique of measuring atomic nitrogen density by monitoring the nitrogen afterglow emission. In a discharge through varying mixtures of H_2 with N_2, it is shown that it is necessary to include the quenching effects of H_2 and H atoms on the $N_2(B^3\Pi_g, v=11)$ state for the afterglow measurements to agree with the N-atom TALIF data.

DETAILED KINETIC MODELING OF POLYCYCLIC AROMATIC HYDROCARBONS IN ETHENE DIFFUSION FLAMES

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The mechanisms by which aromatic compounds are formed in ethene diffusion flames are studied using a detailed chemical kinetic model. Our starting model has previously been tested against measurements in premixed flames and jet-stirred reactors. In the present work, predictions for major species and stable intermediates including aromatics up to pyrene are compared with measurements in counterflow ethene diffusion flames. Preliminary results suggest that, because of differing flame structure, different reaction paths play the principal role in diffusion and premixed flames. Additional reactions involving C_3H_5 and C_3H_6 were necessary to bring C_3H_4 and benzene into agreement with measured values. Predictions for species as large as single-ring aromatics are in quantitative agreement with measured values, while two-ring aromatics are underpredicted by about 50%. Reactions of propargyl and reactions between C_4 and C_2 species contribute to the formation of the first ring. These reactions are highly reversible; the propargyl route is the least reversible and therefore provides the majority of the net production of benzene. Analysis of reaction pathways responsible for growth of larger aromatics is in progress.

EXPERIMENTAL STUDY OF THE STRUCTURE OF SEVERAL NON-SOOTING RICH PREMIXED ACETYLENE FLAMES

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Four low pressure premixed acetylene/oxygen/argon flames with equivalence ratio (ϕ) of 1.00, 1.50, 2.00 and 2.25 have been investigated. The initial percentage of O_2 has been kept identical in all flames to facilitate comparisons between flames. Signal intensity profiles of stable, atomic and radical species were measured by using mass spectrometry coupled with molecular beam sampling. Absolute concentrations have been obtained by an appropriate calibration and by measuring the corresponding temperature profiles in each individual flame by means of a PtRh6%/PtRh30% thermocouple. An increase of the maximum mole fractions of C_3H_3, C_4H_2, C_4H_4 and C_4H_6, with the equivalence ratio is demonstrated.
Rate coefficients of consumption reactions of acetylene with oxygen atoms and hydroxyl radicals have been deduced and compared with the literature data.

$C_2H_2 + O \rightarrow Products$	$k = 5.66 \times 10^{14} \exp(-3061/T)$ ($\phi = 1.00$)
	$k = 4.27 \times 10^{14} \exp(-3331/T)$ ($\phi = 1.50$)
$C_2H_2 + OH \rightarrow CH_3 + CO$	$k = 4.0 \times 10^{13} \exp(-6584/T)$ ($\phi = 1.00$)
	$k = 7.6 \times 10^{13} \exp(-6791/T)$ ($\phi = 1.50$)

Rate coefficients of reactions of H atoms with C_2H_2, C_4H_2, C_4H_4 and C_6H_2 have been determined around 1500 K.

$C_2H_2 + H \rightarrow Products$	$k = 1.78 \times 10^{11}$ cm^3 mol^{-1} s^{-1}
$C_4H_2 + H \rightarrow Products$	$k = 4.10 \times 10^{11}$
$C_4H_4 + H \rightarrow Products$	$k = 1.11 \times 10^{12}$
$C_6H_2 + H \rightarrow Products$	$k = 1.62 \times 10^{12}$

DETERMINATION OF RATE COEFFICIENTS FOR REACTIONS OF FORMALDEHYDE PYROLYSIS AND OXIDATION IN THE GAS PHASE

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Seven mixture of formaldehyde and oxygen diluted in argon were studied behind reflected shock waves at temperatures from 1340 to 2270 K and pressures from 0.7 to 2.5 atm. Formaldehyde was produced by thermal decomposition of its trimer, 1,3,5-trioxane behind the reflected shock front. Mixture compositions were chosen based on preliminary sensitivity analysis and were as follows: Series A, 1.97% CH_2O/Ar; Series B, 1.46% CH_2O/Ar; Series C, 1.47% CH_2O/0.25% O_2/Ar; Series D, 1.00% CH_2O/0.60% O_2/Ar; Series E, 1.50% CH_2O/1.50% O_2/Ar; Series F, 0.49%

CH_2O/1.98% O_2/Ar; Series G, 1.00% CH_2O/5.96% O_2/Ar. The progress of reaction was monitored by infrared laser absorption of CO molecules at (2→1), P(10) transition.

Kinetic information was deduced from the experimental data by matching the initial part of the CO profiles, from the onset of reaction up to the maximum in the absorption signal. Preliminary numerical analysis showed that the remaining part of the CO profiles (that is, after the maximum) was mostly sensitive to the reaction $CO+OH \rightarrow H+CO_2$ and hence did not provide additional information on formaldehyde reactions. Thus, each experimental profile was represented by three characteristic points, $t_{0.25}$, $t_{0.50}$, and $t_{0.75}$, the times at which the CO signal reached 0.25, 0.50 and 0.75 of its maximum value, respectively.

Experimental rates of CO formation were found to be 80% higher, in the case of pyrolysis, and 30% lower, under lean oxidation, than those predicted by the current reaction model, GRI-Mech 1.2. The collected experimental data were subjected to extensive detailed chemical kinetics analysis, including optimization with the solution mapping technique. The analysis identified a strong correlation between two rate constants, k_{1a} and k_2. Assuming a recent literature expression

$$k_2 = 5.74 \times 10^7\ T^{1.9} \exp(-1380/T)\ cm^3\ mol^{-1}\ s^{-1}$$

for

$$H + CH_2O \rightarrow HCO + H_2 \quad (2)$$

produced

$$k_{-1a} = 2.66 \times 10^{24}\ T^{-2.57} \exp(-215/T)\ cm^6\ mol^{-2}\ s^{-1}$$

for

$$H + HCO + M \rightarrow CH_2O + M \qquad (1a)$$

A new expression was developed for

$$HO_2 + CH_2O \rightarrow HCO + H_2O_2 \qquad (6)$$

$$k_6 = 4.11 \times 10^4\ T^{2.5} \exp(-5136/T)\ cm^3\ mol^{-1}\ s^{-1}$$

by fitting the present and literature results. With these modifications, the new reaction model provides good agreement with our experimental data and an acceptable agreement with most literature experimental observations.

Density Functional Studies on the Rate Constants for the Reaction of N_2O with O, OH and CO

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The reactions of N_2O with $O(^3P)$, OH and CO have been studied by ab initio molecular orbital and statistical theoretical calculations. The molecular orbital calculations were performed using the GAUSSIAN 94 program. The Becke's hybrid functional (B3LYP) in density functional methods was used with Dunnings' correlation consistent triple-zeta basis set (cc-pVTZ). Rate constants for the reactions were calculated with conventional transition theory with the Wigner's tunneling correction and compared with experimental data reported previously.

The $N_2O+O(^3P)$ reaction has two products channels, NO+NO and N_2+O_2. Barrier heights for the two competitive pathways were calculated to be 18 and 33 kcal/mol, respectively, including zero-point energy correction. Although comparable values of branching ratio for the product channel have been reported in some experiments by fitting to complex mechanism, this calculation suggested that the first path is favorable. Calculated overall rate constants for this reaction and rate constants for the reverse reaction of the first path, that is, $NO+NO \rightarrow N_2O+O(^3P)$ are consistent with experimental data.

For the N_2O+OH reaction, it was indicated that the products channel of the reaction is N_2+HO_2 and reaction path is not correlated to the products of HNO+NO. Reaction barrier of 35 kcal/mol including zero-point energy correction was found. As far as we have searched, no reliable kinetic data are available.

Experimental rate constant data for the $N_2O+CO \rightarrow N_2+CO_2$ reaction are in disagreement especially in the magnitude of activation energy. The data are divided into two groups; one is with about 19 kcal/mol of the activation energy, the other with about 48 kcal/mol. The present calculation supported the magnitude of the latter. But the calculated pre-exponential factor of the rate constants was found to be much less than those of experimental ones.

It was suggested by this work that rates for the N_2O+OH and N_2O+CO reactions are very slow at around the temperature range of 1000-1500 K, and these reactions are unimportant for the N_2O fate in combustion.

Rates of the $O+N_2O$ Reaction

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The reactions of N_2O with O atoms are critical to models of propellant dark zone combustion and also pertain to models of NO_x pollutant formation. They are:

$O+N_2O \rightarrow NO+NO \quad \Delta H_0=-150$ kJ mol^{-1} (1)

$O+N_2O \rightarrow O_2+N_2 \quad \Delta H_0=-330$ (2)

Critical reviews concluded that the two channels have identical rate coefficients:

$k_1(T)=k_2(T)=1.7\times10^{-10}\exp(-14100\ K/T)\ cm^3\ mol^{-1}\ s^{-1}$ (1200-2000 K)

However, a recent shock tube study yielded a similar result for k_1, but very different results for k_2:

$k_2(T)=2.3\times10^{-12}\exp(-5440\ K/T)\ cm^3\ mol^{-1}\ s^{-1}$ (1940-3340 K)

Extrapolation of either $k_2(T)$ or of $k_t(T)=k_1(T)+k_2(T)$ to the lower temperatures typical of propellant combustion yields results several orders of magnitude larger than previously assumed.

Here we report lower temperature range measurements made at RPI using the High Temperature Photochemistry (HTP) technique, which yield

$k_t(1076\text{-}1276\ K)=2.7\times10^{-9}\exp(-14580\ K/T)\ cm^3\ mol^{-1}\ s^{-1}$

A critical review of the voluminous literature and fitting of the best results, which include the new RPI measurements, has been conducted by the ARL authors, resulting in new recommendations.

The HTP work represents the first measurements on the overall reaction under conditions in which results are well isolated from effects of other reactions. Thus, there is no dependence of the results on ancillary kinetic data, as in prior studies. The possible influence of H_2O on the reactions, suggested in other studies, was modeled. The modeling predictions indeed indicate the results would be highly sensitive to even a few ppm of H_2O impurities. However, measurements of the apparatus' leak rate show that the possible H_2O impurity concentrations must have been negligibly low. The new measurements concur with the shock tube measurements in that the rate coefficients below 1700 K are much larger than previously thought, but they indicate that the value at 1100 K is about 2.5 times lower than extrapolation of the previous results.

The ARL model is based on a state-of-the-art detailed mechanism for the dark zones of solid propellants consisting of ≈200 reactions. The appropriate subsets of reactions were extracted from this mechanism and used for the simpler mixtures encountered in the present work. The best rate coefficient information currently available was used without alteration except, of course, rate coefficients for the title reaction were varied. Detailed chemical modeling, mimicking typical conditions described in the various experiments, was done to test assumptions used for determination of k_1 and k_2. There were three major reasons found for rejection of a given data set from the fitted results: (i) discovery of invalid assumptions, foremost amongst these being important errors concerning the chemical mechanism, (ii) usage of low purity reactants, and (iii) proof that although the mechanism used to model results was essentially correct (matches results well), the results are not very sensitive to the title reaction. The results were fitted to obtain the recommendations for k_1 and k_2:

$k_1(T) = 1.7 \times 10^{-10} \exp(-14100\ K/T)\ cm^3\ mol^{-1}\ s^{-1}$ (1370-3850 K)

$k_2(T) = 6.1 \times 10^{-12} \exp(-8000\ K/T)\ cm^3\ mol^{-1}\ s^{-1}$ (1076-3340 K)

The results for k_1 agree with most prior works. The results for k_2 are much larger below 1700 K than the reviews suggest.

PHOTOFRAGMENT TRANSLATIONAL SPECTROSCOPY OF $C_3H_3X(X=Cl,Br,H)$

W. Sun, K. Yokoyama, J. Robinson and D. Neumark, University of California, Berkeley, CA, and N. Hemmi, Lawrence Berkeley National Laboratory (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

Propargyl chloride, $HCCCH_2Cl$, propargyl bromide, $HCCCH_2Br$ and allene, H_2CCCH_2, are photolyzed by a 193 and 248 nm excimer laser to produce propargyl radical, H_2CCCH, with a crossed laser-molecular beam apparatus. Photofragments are ionized in a quadrupole mass spectrometer by energy-controlled photons from an advanced light source. In the case of 193 nm photolysis of propargyl chloride, C_3H_2 has been found to have two components in its TOF spectra. The faster component can be assigned as photofragments from a secondary photodissociation of propargyl radical to produce H atom and C_3H_2. The ionization potential of the C_3H_2 fast component has been measured to be below 10 eV. This indicates that its structure is not $H_2C=C=C$ whose IP was reported to be around 10.4 eV. Results of photolysis of the other species and at 248 nm will be presented at this meeting.

EXPERIMENTAL AND THEORETICAL DYNAMICS OF $O(^3P)$ ATOM REACTIONS WITH SULFUR-CONTAINING COMPOUNDS

B.R. Weiner, Department of Chemistry, University of Puerto Rico, P.O. Box 23346, UPR Station, Rio Piedras, Puerto Rico 00931 (Presented at the *1998 Joint Meeting of the American Physical Society and the American Association of Physics Teachers*, Held in Columbus OH, April 1998).

The detailed dynamics of $O(^3P)$ atom reactions with sulfur compounds (OCS, CS_2, C_2H_4S, CH_3SH and $CSCl_2$) have been studied experimentally by measuring the nascent $SO(X^3\Sigma^-)$ product rovibrational energy distributions, and computationally by determining the optimized geometries of the possible reaction intermediates. Some of the reactions have important implications in the global sulfur budget and radiation balance. Ground state $O(^3P)$ atoms are generated by photolysis of NO_2 either by the 351 nm output from a XeF excimer laser or the 355 nm output from a frequency tripled Nd-YAG laser. The $SO(X^3\Sigma^-)$ product from the reactions is monitored by measuring the laser induced fluorescence signal on the $(B^3\Sigma^- - X^3\Sigma^-)$ transition in the wavelength region of 237-312 nm. The observed vibrational distributions vary from statistical to inverted and are used to determine the mechanisms of the above reactions. Franck-Condon and statistical energy disposal models are used to simulate the nascent energy distributions and support the proposed mechanisms. Ab initio correlated calculations at the complete fourth-order Moller-Plesset theory (MP4 SDTQ/6-311+G*) have been performed in order to determine the structures and relative stabilities of the proposed reactive intermediates as well as the relative energetics of the reactants and products. The collaborative experimental and theoretical effort has led to a greater understanding of the reaction dynamics of these systems.

CONTROLLING DISSOCIATION PATHWAYS AND WATCHING ENERGY FLOW IN VIBRATIONALLY EXCITED MOLECULES

F.F. Crim, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706
(Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

Controlling chemical reactions using lasers is a conceptually simple notion that has proven challenging in practice. Such control requires a detailed understanding of the initial state that vibrational excitation creates and of the electronically excited state in which dissociation occurs. Vibrationally mediated photodissociation provides the first examples of vibrational state control to produce bond-selected chemistry. In these experiments, one laser prepares a vibrationally excited molecule, another dissociates the molecule by electronic excitation, and a third probes the products to determine their identity and quantum state populations. It is also possible to perform time resolved vibrationally mediated photodissociation experiments using ultrafast lasers in order to observe the intramolecular redistribution of energy in vibrationally excited molecules. In such measurements, the electronically excited surface is a window into the dynamics on the ground electronic state. Preparing a molecular eigenstate with one laser and subsequently turning that stationary state into a dissociative one by electronic excitation is a proven means of controlling the dissociation pathways in a triatomic molecule, HOD. The same approach controls bond cleavage in a tetra-atomic molecule, HNCO, in which the two product channels, producing either NH+CO or H+NCO, are chemically rather than isotopically distinct. An understanding of the nature of the initially prepared vibrational states and their influence on the photodissociation allows one to invert the process and use the dissociation step as a probe of vibrational dynamics in the ground electronic state. The most recent experiments use ultrafast excitation of the O-H stretching vibration in nitric acid ($HONO_2$) with a 100 fs laser pulse and subsequent photodissociation with another 100 fs pulse to follow the transfer energy out of the coherently excited O-H stretching motion.

LASER ABLATION MECHANISM OF ALKALINE EARTH METALS

H. Nishikawa, M. Kanai and T. Kawai, ISIR-Sanken, Osaka University, Japan (Presented at the *1998 March Meeting of the American Physical Society*, Held in Los Angeles CA, March 1998).

In order to understand the nascent process of laser ablation of metals, the amount of desorbed monovalent ions have been measured on the laser ablation of alkaline earth metals. The relationship between the amount of the desorbed ion and the laser fluence is $I^{4.6(\pm 0.2)}$, $I^{3.7(\pm 0.4)}$ and $I^{2.9(\pm 0.3)}$ for Ca, Sr and Ba, respectively, when ArF excimer laser (6.4 eV, 193 nm) is used as a light source. Here, I represents the laser fluence. The results can be interpreted that the desorption is caused by 5-, 4- and 3-photon process for Ca, Sr and Ba, respectively, because such nonlinear behavior is caused by a certain multiphoton process. Since the total photon energy of 3-, 4- and 5-ordered processes correspond to the highest core electron level for each metal, a model has been proposed that the laser ablation of the alkaline earth metal is triggered by excitation of the outermost core electron. The experiment using KrF excimer laser (5.0 eV, 248 nm) has been performed to give more evidence for the above mentioned model. The relationship between the amount of desorbed ion and the laser fluence is $I^{6.4(\pm 1.0)}$, $I^{5.3(\pm 1.2)}$ and $I^{3.6(\pm 1.0)}$ for Ca, Sr and Ba, respectively. Such values also correspond to the outermost core level of each metal.

AB INITIO AND DFT POTENTIAL ENERGY SURFACES FOR CYANURIC CHLORIDE REACTIONS

S.V. Pai, C.F. Chabalowski and B.M. Rice, Weapons and Materials Research Directorate, Army Research Laboratory, Aberdeen Proving Ground, MD 21005 (Army Research Laboratory Final Report ARL-TR-1718 , 37 pp., July 1998).

Ab initio and nonlocal density functional theory (DFT) calculations were performed to determine reaction mechanisms for formation of the six-membered ring $C_3N_3Cl_3$ (cyanuric chloride) from the monomer, cyanogen chloride (ClCN). MP2 geometry optimizations followed by QCISD(T) energy refinements and corrections for zero-point energies for critical points on the potential energy surface were calculated using the 6-31G and 6-311+G basis sets. DFT(B3LYP) geometry optimizations and zero-point corrections for critical points on the potential energy surface were calculated with the 6-31G, 6-311+G, and cc-pVTZ basis sets. Two formation mechanisms of cyanuric chloride were investigated, the concerted triple association (3 ClCN$\rightarrow$cyanuric chloride) and the step-wise association (3 ClCN$\rightarrow Cl_2C_2N_2$+ClCN$\rightarrow$cyanuric chloride). All calculations show that the lower energy path to formation of cyanuric chloride is the concerted triple association. MP2 and DFT intrinsic reaction coordinate (IRC) calculations starting from the transition state (TS) for concerted triple association reaction proceeding toward the isolated monomer resulted in the location of a local minimum, stable by as much as -8.0 kcal/mol, that corresponds to a weakly bound cyclic $(ClCN)_3$ cluster. The existence of this cluster on the reaction path for the concerted triple association could lower the entropic hindrance to this unusual association reaction mechanism.

MODELING OF VIBRATION-TO-VIBRATION AND VIBRATION-TO-ELECTRONIC ENERGY TRANSFER PROCESSES IN OPTICALLY PUMPED PLASMAS

I.V. Adamovich, E. Ploenjes, P. Palm and J.W. Rich, Department of Mechanical Engineering, The Ohio State University, Columbus OH, and A. Chernukho, A.V. Lykov Heat and Mass Transfer Institute, Minsk, Belarus (Presented at the *51st Annual Gaseous Electronics Conference and the 4th International Conference on Reactive Plasmas*, Held in Maui HI, October 1998).

The paper presents the results of modeling of the optical pumping experiments in $CO/N_2/O_2$/Ar mixtures. In these experiments, the low vibrational levels of carbon monoxide ($v<12$) are excited by resonant absorption of the CO laser radiation. The high vibrational levels, up to $v=40$, are populated by the CO-CO vibration-to-vibration (V-V) energy exchange. Time-resolved CO infrared and ultraviolet radiation from the excited electronic states is measured by a high-resolution step-scan Fourier transform spectrometer. The kinetic model incorporates coupled master equation for the CO, N_2 and O_2 vibrational level populations, and Boltzmann equation for the electrons. The comparison of the experimental and synthetic time-resolved spectra allowed inference of the V-V exchange rates for CO-CO up to $v=40$, cross sections for the energy transfer between the highly excited CO molecules and electrons, and V-V transfer rates for CO-N_2 and CO-O_2 .

VAPOR PRESSURE OF CESIUM BETWEEN 270 AND 370 K VIA LASER ABSORPTION

R.J. Rafac and C.E. Tanner, University of Notre Dame, Notre Dame IN (Presented at the *1998 Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*, Held in Santa Fe NM, May 1998).

For more than sixty years, experimenters have relied on the vapor pressure equations from Taylor and Langmuir's positive ion measurements to calibrate the densities of saturated atomic cesium vapor for numerous spectroscopic applications. We update these results with additional data obtained via measurement of the direct absorption of narrow-band laser radiation nearly resonant with the ground state to $6^2P_{3/2}$ transition. The Doppler broadened transmission of a cesium vapor cell is recorded for several GHz of detuning using a high-precision absorption spectrometer. Complementary measurements of the collisional broadening of the resonance lines and laser spectral composition are also performed, which in concert with high precision transition strength data permit the accurate calculation of the absorption profile of the vapor. In this fashion the absolute vapor densities at various temperatures are determined and related to the observed transmission spectra. Good agreement is established with the early experiments. These measurements also allow the determination of the heat of sublimation of cesium at absolute zero, 76.5(1) kJ/mol.

CURRENT BIBLIOGRAPHY RELEVANT TO FUNDAMENTAL COMBUSTION

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Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797
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1. FUELS/SYNFUELS - GENERAL

77657. Flecher, P.E., W.T. Welch, S. Albin and J.B. Cooper, "Determination of Octane Numbers and Reid Vapor Pressure in Commercial Gasoline Using Dispersive Fiber Optic Raman Spectroscopy," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 199-206 (1997).
Gasoline
Octane Number
Raman Spectral Monitoring Method

2. LIQUEFACTION/GASIFICATION

77658. Ergudenler, A., A.E. Ghaly, F. Hamdullahpur and A.M. Al-Taweel, "Mathematical Modeling of a Fluidized Bed Straw Gasifier. I. Model Development," *Energy Sources* 19, 1065-1084 (1997).
Gasifier
Fluidized Bed
Straw Fuels
Model

77659. Ergudenler, A., A.E. Ghaly, F. Hamdullahpur and A.M. Al-Taweel, "Mathematical Modeling of a Fluidized Bed Straw Gasifier. II. Model Sensitivity," *Energy Sources* 19, 1085-1098 (1997).
Gasifier
Fluidized Bed
Straw Fuels
Model Testing

77660. Ergudenler, A., A.E. Ghaly, F. Hamdullahpur and A.M. Al-Taweel, "Mathematical Modeling of a Fluidized Bed Straw Gasifier. III. Model Verification," *Energy Sources* 19, 1099-1121 (1997).
Gasifier
Fluidized Bed
Straw Fuels
Model Validation

3. BURNERS

77661. Kennedy, L.A., A.A. Fridman and A.V. Saveliev, "Superadiabatic Combustion in Porous Media: Wave Propagation, Instabilities, New Type of Chemical Reactor," *Fluid Mech. Res.* 22(2), 1-26 (1995).
Porous Burner Combustion
CH_4, C_2H_2, H_2
Propagation
Superadiabatic Temperatures
Stabilities

77662. Mulder, A., O. Brost and P. Neumann, "Catalytic Combustion in a Sintered Metal Reactor with Integrated Heat Exchanger," *Appl. Thermal Eng.* 17, 825-836 (1997).
Sintered Metal Burner
CH_4
Catalytic Combustion
CO,NO Emissions
Model

77663. Bhidayasiri, R., S. Sivasegaram and J.H. Whitelaw, "The Effect of Flow Boundary Conditions on the Stability of Quarl-Stabilized Flames," *Combust. Sci. Technol.* 123, 185-205 (1997).

Quarl Burners
Swirl
Stabilization
Limits
Oscillations

77664. Knoop, P., F.E.C. Culick and E.E. Zukoski, "Extension of the Stability of Motions in a Combustion Chamber by Nonlinear Active Control Based on Hysteresis," *Combust. Sci. Technol.* 123, 363-376 (1997).

Dump Combustor
Instabilities
Hysterisis
Active Control
Method

(77784) Weak Fuel Jet/Strong Air Jet Interactions, Flowfield

Low NO_x Burner

77665. Gil, Y.S., H.S. Jung and S.H. Chung, "Premixed Flame Stabilization in an Axisymmetric Curved-Wall Jet," *Combust. Flame* 113, 348-357 (1998).

Curved Wall
Jet Burner
LDV
Flowfield
Blow-off
Flame Length
Stabilization

77666. Stenberg, J., L.-E. Amand, R. Hernberg and B. Leckner, "Measurements of Gas Concentrations in a Fluidized Bed Combustor Using Laser Induced Photoacoustic Spectroscopy and Zirconia Cell Probes," *Combust. Flame* 113, 477-486 (1998).

FBC
Coal,Peat
Wood Chips
Optoacoustic
NO,SO_2
Monitoring

4. COAL, PARTICLE COMBUSTION/PYROLYSIS

77667. Faltsi-Saravelou, O., P. Wild, S.S. Sazhin and J.E. Michel, "Detailed Modeling of a Swirling Coal Flame," *Combust. Sci. Technol.* 123, 1-22 (1997).

Coal Flame
Swirling
Species Transport
Combustion Kinetics
T,Species Profiles
Flowfield
Modeling

77668. Peters, A.A.F., and R. Weber, "Mathematical Modeling of a 2.4 MW Swirling Pulverized Coal Flame," *Combust. Sci. Technol.* 122, 131-182 (1997).

Pulverized Coal
Swirling
Turbulent Flame
NO Formation
Numerical Model

(77666) FBC, NO, SO_2 Optoacoustic Monitoring

Coal,Peat
Woodchips

77669. Pedersen, L.S., P. Breithaupt, K. Dam-Johansen and R. Weber, "Residence Time Distributions in Confined Swirling Flames," *Combust. Sci. Technol.* 127, 251-273 (1997).

Pulverized Coal
Swirling Flames
Residence Times
Distributions

(77728) Ignition, Shock Tube, Numerical Analysis — Coal Particles

77670. Reddy, P.D., P.R. Amyotte and M.J. Pegg, "Effect of Inerts on Layer Ignition Temperatures of Coal Dust," *Combust. Flame* 114, 41-53 (1998).
Coal Dust
Ignition
Temperatures
Hot Surface
Dolomite,Limestone
Admixture Effects

77671. Wu, Z., L. Xu, Z. Wang and Z. Zhang, "Catalytic Effects on the Ignition Temperature of Coal," *Fuel* 77, 891-893 (1998).
Coal
Ignition
Temperatures
Salt Catalysis
Metal IP,
H_2O Effects

77672. Reinelt, D., A. Laurs and G. Adomeit, "Ignition and Combustion of a Packed Bed in a Stagnation Point Flow. II. Heterogeneous and Homogeneous Reactions," *Combust. Flame* 113, 373-379 (1998).
Carbon
Packed Bed
Stagnation
Point Flow
Gas/Solid
Combustion
Simulation

77673. Borovinskaya, I.P., S.G. Vadchenko and A.G. Merzhanov, "High Temperature Oxidation of Carbon Filaments," *Dokl. Phys. Chem.* 350, 243-245 (1996).
Carbon Filament
Oxidation
Rates

77674. Zhang, X., A. Dukhan, I.I. Kantorovich and E. Bar-Ziv, "The Thermal Conductivity and Porous Structure of Char Particles," *Combust. Flame* 113, 519-531 (1998).
Char Particles
Thermal
Conductivity
2 Measurement
Methods

77675. Kantorovich, I.I., and E. Bar-Ziv, "Role of the Pore Structure in the Fragmentation of Highly Porous Char Particles," *Combust. Flame* 113, 532-541 (1998).
Char Particles
Combustion
Fragmentation
Porosity
Dependence

77676. Ouedraogo, A., J.C. Mulligan and J.G. Cleland, "A Quasi-Steady Shrinking Core Analysis of Wood Combustion," *Combust. Flame* 114, 1-12 (1998).
Wood Particle
Combustion
Shrinking Core
Model

77677. Lightstone, M.F., and G.D. Raithby, "A Stochastic Model of Particle Dispersion in a Turbulent Gaseous Environment," *Combust. Flame* 113, 424-441 (1998).
Particle
Dispersion
Turbulent
Gaseous Flowfields
Model

5. SPRAY COMBUSTION

(See also Section 23 for Droplet Characterization)

77678.	D'Alessio, A., F. Beretta, P. Massoli and M. Lazzaro, "Thermal Stability, Atomization and Spray Combustion of Fuel Oils," pp. 317-351 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Fuel Oil Spray Atomization Combustion Scattering Measurements Sizes
77679.	Gomez, A., and G. Chen, "Monodisperse Electrosprays: Combustion, Scale-up and Implications for Pollutant Formation," pp. 461-505 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Spray Combustion Electrostatic Dispersion Size Effects Soot Formation
77680.	Gupta, A.K., C. Presser, J.T. Hodges and C.T. Avedisian, "Role of Combustion on Droplet Transport in Pressure-Atomized Spray Flames," Presented Originally as AIAA Paper 94-0115 at the *32nd AIAA Aerospace Sciences Meeting and Exhibit*, Held in Reno NV, January 1994, *J. Propulsion Power* 12, 543-553 (1996).	Spray Flames Kerosene Sizes,Velocities Transport
77681.	Zuo, B., and E. Van Den Bulck, "A Quasi-Global Mechanism for Oxidation of Fuel Oil and the Laminar Flame Data Library," *Combust. Flame* 113, 615-619 (1998).	Fuel Oil Combustion Prevaporized Premixed Quasi-Global Mechanism Kinetic Modeling
77682.	Schiller, D., J. Li and W.A. Sirignano, "Transient Heating, Gasification and Oxidation of an Energetic Liquid Fuel," *Combust. Flame* 114, 349-358 (1998).	Energetic Liquid Fuel Droplet Gasification Oxidation Mechanism Model
77683.	Duvvur, A., C.H. Chiang and W.A. Sirignano, "Oscillatory Fuel Droplet Vaporization: Driving Mechanism for Combustion Instability," *J. Propulsion Power* 12, 358-365 (1996).	Droplet Vaporization Driven Instabilities Modeling
77684.	Aggarwal, S.K., and M. Mawid, "Fuel Vapor Accumulation Effect on the Combustion Characteristics of Multicomponent Fuel Droplets," *Chem. Eng. Commun.* 157, 35-51 (1997).	Fuel Droplet Combustion Multicomponent Vapor Accumulation Effects Modeling
(77897)	$C_6H_5CH_3/CH_3OH$ Droplet Combustion, Microgravity, Soot Shells	Soot Formation

77685. Aharon, I., and B.D. Shaw, "Estimates of Liquid Species Diffusivities from Experiments on Reduced Gravity Combustion of Heptane/Hexadecane Droplets," *Combust. Flame* 113, 507-518 (1998).

Droplet
Combustion
$C_7H_{16}/C_{16}H_{34}$
Reduced Gravity
Liquid Species
Diffusion
Coefficients

6. METALS/PROPELLANTS/POLYMER COMBUSTION

77686. Novozhilov, B.V., "Two-Dimensional Approximation in the Theory of Surface Spin Combustion," *Dokl. Phys. Chem.* 341, 56-58 (1995).

Spin Combustion
Cylindrical
Metal Sample
Gas/Surface
Model

77687. Carotenuto, L., G. Continillo and S. Crescitelli, "Propagation of Gasless Combustion Fronts: Nonzero Reaction Rate in the Whole Domain," *Chem. Eng. Commun.* 145, 173-193 (1996).

Solid Phase
Combustion
Propagation
Modeling

77688. Volpert, Vl.A., and Vit.A. Volpert, "Condensed Phase Reaction Waves with Variable Thermophysical Characteristics," *Combust. Sci. Technol.* 127, 29-53 (1997).

Solid Phase
Combustion
Propagation
Stability

77689. Grachev, V.V., and T.P. Ivleva, "Filtration Combustion in the Closed Volume of a Self Propagating High Temperature Synthesis Reactor," *Combust. Expl. Shock Waves, Russia* 33, 539-547 (1997).

Solid Phase
Combustion
Cylindrical Vessel
Propagation
Model

77690. Shkadinsky, K.G., G.V. Shkadinskaya and B.J. Matkowsky, "Ignition of Heterogeneous Mixtures in Gravitational Fields," *Combust. Flame* 113, 388-405 (1998).

Solid Phase
Combustion
Ignition
Melting/
Sedimentation
Gravitational
Role
Model

77691. Williams, F.A., "Some Aspects of Metal Particle Combustion," pp. 267-288 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).

Metal Particles
Al,B,C.Mg
Combustion
Review

77692. Puszynski, J.A., S. Majorowski and V. Hlavacek, "Densification of Aluminum Nitride-Based Ceramic Materials Synthesized by Combustion of Aluminum in Air," *Chem. Eng. Commun.* 152/153, 75-85 (1996).

Al(s)/Air
Combustion
AlN Formation

(77776)	Deflagration/Detonation Transition, End Wall Pressures	Al Dust/C_2H_2/Air
77693.	Frolov, Yu.V., and A.N. Pivkina, "Fractal Structure and Features of Energy Release (Combustion) Processes in Heterogeneous Condensed Systems," *Combust. Expl. Shock Waves, Russia* 33, 513-527 (1997).	Solid Phase Combustion Al/Ni,Zr,Fe_2O_3 Al,Ni/AP/PMMA Fractal Theory Application
77694.	Simonyan, A.V., V.A. Gorshkov and V.I. Yukhvid, "Combustion of the NiO/Al System under Gas Pressure," *Combust. Expl. Shock Waves, Russia* 33, 528-531 (1997).	Solid Phase Combustion Al/NiO Gas Pressure Control NiAl Product
77695.	Yuasa, S., T. Yoshida, M. Kawashima and H. Isoda, "Effects of Pressure and Oxygen Concentration on Ignition and Combustion of Boron in Oxygen/Nitrogen Mixture Streams," *Combust. Flame* 113, 380-387 (1998).	B(s)/O_2/N_2 Ignition Combustion Pressure,O_2 Effects
77696.	Hwang, S., A.S. Mukasyan, A.S. Rogachev and A. Varma, "Combustion Wave Microstructure in Gas/Solid Reaction Systems: Experiments and Theory," *Combust. Sci. Technol.* 123, 165-184 (1997).	Ti(s)/N_2 Combustion Propagation Wave Front Fluctuations
77697.	Baker, P.J., and A.M. Mellor, "Energetic Materials Impact Initiation Mechanisms," pp. 289-316 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Energetic Materials Impact Ignition Mechanisms Review
77698.	Ulas, A., and K.K. Kuo, "Effect of Aging on Ignition Delay Times of a Composite Solid Propellant Under CO_2 Laser Heating," *Combust. Sci. Technol.* 127, 319-331 (1997).	Solid Propellants Ignition Delays IR Laser Heating Aging Effects
77699.	Fell Jr, N.F., J.A. Vanderhoff, R.A. Pesce-Rodriguez and K.L. McNesby, "Characterization of Raman Spectral Changes in Energetic Materials and Propellants During Heating," *J. Raman Spectrosc.* 29, 165-172 (1998).	Energetic Materials Explosives Heating Effects Raman Monitor
77700.	Margolis, S.B., "Hydrodynamic Instability in an Extended Landau/Levich Model of Liquid Propellant Combustion at Normal and Reduced Gravity," *Combust. Flame* 113, 406-423 (1998).	Liquid Propellant Combustion Hydrodynamic Instabilities Model
77701.	Schmitt, R.G., P.B. Butler and J.J. Freesmeier, "Performance and CO Production of a Non-Azide Airbag Propellant in a Pre-Pressurized Gas Generator," *Combust. Sci. Technol.* 122, 305-330 (1997).	Solid Propellant Airbag Inflator Method CO Chemistry

77702. Hites, M.H., and M.Q. Brewster, "Effects of Kevlar Fibers on Ammonium Perchlorate Propellant Combustion," *J. Propulsion Power* 12, 616-619 (1996).

Propellant
AP
Combustion
Kevlar Fiber
Burning Rate
Enhancements

(78388) Equilibrium Calculations, Combustion, Method

JPN Propellant

77703. Fetherolf, B.L., and T.A. Litzinger, "CO_2 Laser Induced Combustion of Ammonium Dinitramide, ADN," *Combust. Flame* 114, 515-530 (1998).

$NH_4N(NO_2)_2$
Laser Ignition
Gaseous Species
Probe Sampling
Mass Analysis

77704. Williams, G.K., and T.B. Brill, "Thermal Decomposition of Energetic Materials. LXII. Unusual Behavior of Substituted Furazan Compounds upon Flash Pyrolysis," *Combust. Flame* 114, 569-576 (1998).

Energetic Materials
c-$RR'C_2N_2O$
Pyrolysis
Product
IR,Mass Analysis

77705. Ward, M.J., S.F. Son and M.Q. Brewster, "Steady Deflagration of HMX with Simple Kinetics: A Gas Phase Chain Reaction Model," *Combust. Flame* 114, 556-568 (1998).

HMX
Combustion
Chain Reaction
Mechanism
Burning Rates
Model

77706. Lu, Y.-C., A. Ulas, E. Boyer and K.K. Kuo, "Determination of Temperature Profiles of Self-Deflagrating RDX by Ultraviolet/ Visible Absorption Spectroscopy and Fine-Wire Thermocouples," *Combust. Sci. Technol.* 123, 147-163 (1997).

RDX
Self-Deflagrating
Temperature
Profiles
Thermocouple
Absorption
Measurements

77707. Li, S.C., and F.A. Williams, "Nitramine Deflagration: Reduced Chemical Mechanism for Primary Flame Facilitating Simplified Asymptotic Analysis," *J. Propulsion Power* 12, 302-309 (1996).

RDX,$(CH_2NNO_2)_3$
Deflagration
Velocities
Primary Flame
Kinetic Modeling

77708. Mallery, C.F., and S.T. Thynell, "Species and Temperature Profiles of Propellant Flames Obtained from FTIR Absorption Spectroscopy," *Combust. Sci. Technol.* 122, 113-129 (1997).

RDX
Propellant Flames
T,Species
Profiles
FTIR Absorption

77709. Brewster, M.Q., and T.B. Schroeder, "Laser-Recoil Combustion Response of RDX," *Combust. Sci. Technol.* 122, 363-381 (1997).
RDX
Oscillatory
Combustion Rates
Near Surface
Temperatures
Measurements

77710. Staggs, J.E.J., "A Theoretical Investigation into Modeling Thermal Degradation of Solids Incorporating Finite-Rate Kinetics," *Combust. Sci. Technol.* 123, 261-285 (1997).
Polymer
Solid Combustion
Thermal
Degradation
Pyrolysis
Model

(77910) Fullerenes, AB-Graphitic Structures Formation
Polymer
Combustion

(78098) IR Laser Pyrolysis, Regression Rate, Surface Temperature, Activation Energy
Polybutadiene

77711. Chao, Y.H.C., and A.C. Fernandez-Pello, "Forced Ignition of a Solid Fuel in a Turbulent Boundary Layer Oxidizing Flow," pp. 409-431 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).
PMMA
Heating
Ignition
Boundary Layer
Flows
Turbulence Effects

77712. Novozhilov, V., D.J.E. Harvie, A.R. Green and J.H. Kent, "A Computational Fluid Dynamic Model of Fire Burning Rate and Extinction by Water Sprinkler," *Combust. Sci. Technol.* 123, 227-245 (1997).
PMMA Fires
Burning Rates
Water Spray
Extinction
CFD Model

7. CATALYTIC COMBUSTION

77713. Boehman, A.L., J.W. Simons, S. Niksa and J.G. McCarty, "Dynamic Stress Formation During Catalytic Combustion of Methane in Ceramic Monoliths," *Combust. Sci. Technol.* 122, 257-303 (1997).
Catalytic
Combustion
CH_4
Ceramic Monoliths
Thermal Stress
Analysis

(77662) Catalytic Combustion, Sintered Metal Burner, CO, NO Emissions, Model
CH_4/Air

77714. Au, C.-T., M.-S. Liao and C.-F. Ng, "A Detailed Theoretical Treatment of the Partial Oxidation of Methane to Syngas on Transition and Coinage Metal (M) Catalysts (M=Ni,Pd,Pt,Cu)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3959-3969 (1998).
Catalytic
Partial
Oxidation
CH_4/O_2/Metal
Theoretical
Modeling

77715. Elokhin, V.I., and E.I. Latkin, "Statistical Model of Oscillation and Wave Effects on the Surface of a Catalyst in the Reaction of CO Oxidation," *Dokl. Phys. Chem.* 344, 209-214 (1995).

Catalytic Oxidation
CO/O_2
Oscillations
Model

77716. Kuzovkov, V.N., O. Kortluke and W. von Niessen, "Kinetic Oscillations in the Catalytic CO Oxidation on Pt Single Crystal Surfaces: Theory and Simulation," *J. Chem. Phys.* 108, 5571-5580 (1998).

Catalytic Oxidation
$CO/O_2/Pt$
Kinetic Oscillations
Sticking Coefficient Role

77717. Her, T.-H., R.J. Finlay, C. Wu and E. Mazur, "Surface Femtochemistry of $CO/O_2/Pt(111)$: The Importance of Nonthermalized Substrate Electrons," *J. Chem. Phys.* 108, 8595-8598 (1998).

Catalytic Oxidation
$CO/O_2/Pt$
ps Laser Induced
Nonthermal Electron Role

77718. Saracco, G., J.W. Veldsink, G.F. Versteeg and W.P.M. van Swaaij, "Catalytic Combustion of Propane in a Membrane Reactor with Separate Feed of Reactants. III. Role of Catalyst Load on Reactor Performance," *Chem. Eng. Commun.* 147, 29-42 (1996).

Catalytic Combustion
C_3H_8/Air
Membrane Reactor
Performance

77719. Barelko, V.V., Yu.E. Volodin and E.S. Gen'kin, "Catalytic Emission of Charged Particles in the Course of Ammonia Oxidation on Platinum," *Dokl. Phys. Chem.* 341, 63-65 (1995).

Catalytic Oxidation
$NH_3/O_2/Pt$
Charged Particle Role

77720. Tomishko, M.M., I.A. Nevskii, V.S. Beskov and A.V. Putilov, "Plasma in a Zone of Catalytic Oxidation," *Dokl. Phys. Chem.* 341, 59-62 (1995).

Catalytic Oxidation
$SO_2/Air/Fe_2O_3$
Charged Particle Role

8. MHD

9. TEMPERATURES

(77661) Temperatures, Porous Burner Combustion, CH_4, C_2H_2, H_2 Fuels, Propagation, Stabilities

Superadiabatic

(77709) Near Surface Temperatures, RDX Oscillatory Combustion Rates, Measurements

Thermocouples

(77706)	Temperature Profiles, RDX Self-Deflagrating, Measurements	Thermocouple/ Absorption
77721.	Block, B., W. Hentschel and W. Ertmer, "Pyrometric Determination of Temperature in Rich Flames and Wavelength Dependence of Their Emissivity," *Combust. Flame* 114, 359-369 (1998).	Temperatures Pyrometry Rich Flame Luminosity Emissivity Measurements Method
(78098)	Surface Temperatures, IR Laser Pyrolysis of Polybutadiene, Regression Rates, Activation Energy	Optical Pyrometry
(77708)	Temperature, Species Profiles, RDX Propellant Flames	FTIR Absorption
77722.	Glumac, N.G., "Flame Temperature Predictions and Comparison with Experiment in High Flow Rate, Fuel-Rich Acetylene/Oxygen Flames," *Combust. Sci. Technol.* 122, 383-398 (1997).	Temperatures LIF C_2H_2/O_2 Measurements Kinetic Modeling Discrepancies Flow Rate Effects
(77769)	Temperatures, OH LIF, Imaging, Turbulent CH_4, CH_3OH, C_2H_5OH Diffusion Flames	Rayleigh

10. IGNITION

77723.	Griffiths, J.F., and C. Mohamed, "Experimental and Numerical Studies of Oxidation Chemistry and Spontaneous Ignition Phenomena," Chapter 6 in *Low Temperature Combustion and Autoignition*, M.J. Pilling, ed., 7 Chapters, 794 pp., *Comprehensive Chemical Kinetics* 35, 545-660 (1997).	Auto-ignition Hydrocarbons Mechanisms Modeling Review
77724.	Walker, R.W., and C. Morley, "Basic Chemistry of Combustion," Chapter 1 in *Low Temperature Combustion and Autoignition*, M.J. Pilling, ed., 7 Chapters, 794 pp., *Comprehensive Chemical Kinetics* 35, 1-124 (1997).	Auto-ignition Low Temperature Combustion Cool Flames Alkane,-ene Kinetic Mechanisms Review
(78248)	CO, H_2, Hydrocarbons/O_2, Oscillatory Kinetics, Nonlinear Mathematics, Review	Auto-ignition
77725.	Blumenthal, R., K. Fieweger, K.H. Komp and G. Adomeit, "Gas Dynamic Features of Self-Ignition of Non-Diluted Fuel/Air Mixtures at High Pressure," Reprint (Due to Publishing Errors), Originally Published in *Combust. Sci. Technol.* 113/114, 137-166 (1996) (Bulletin #97, Reference 69437), *ibid.* 123, 389 (1997).	Auto-ignition *n*-C_7H_{16}/Air *i*-C_8H_{18},H_2/Air Delay Times Shock Tube

(78093)	Ignition Delays, Kinetic Modeling, Sensitivity Analysis, Data Comparisons	n-C_7H_{16}/O_2
(78253)	Fuel Knocking Tendencies, n-C_7H_{16}/O_2, Jet Stirred Reactor, Species Profiles, MTBE, ETBE Additive Effects	Auto-ignition
(77838)	I.C. Engines, Pressure Pulses, Predictive Models, Review	Auto-ignition
(77843)	Diesel Engine, Natural Gas Fueled, CFD/Kinetic Modeling	Auto-ignition
77726.	Gel'fand, B.E., S.P. Medvedev, S.V. Khomik, O.E. Popov, A.Yu. Kusharin and G.L. Agafonov, "Self-Ignition of Hydrogen/Oxygen Mixtures at High Initial Pressures," *Dokl. Phys. Chem.* 349, 183-186 (1996).	Self-Ignition H_2/O_2 High Pressure Ignition Delays Discrepancies Shock Tube
77727.	Aivazyan, R.G., "Critical Conditions of Monosilane Self-Ignition with Oxygen and Chain Branching Ratios," *Kinet. Catal., Russia* 38, 174-184 (1997).	Self-Ignition Limits SiH_4/O_2 Chain Branching Mechanism
(77690)	Ignition/Combustion, Melting/Gravitational Sedimentation Role, Model	Heterogeneous Solid Mixtures
(77695)	Ignition, Small Lumps, Pressure, O_2 Effects	$B(s)/O_2/N_2$
77728.	Kiselev, S.P., and V.P. Kiselev, "Ignition of Pulverized Coal Particles in Shock Waves," *J. Appl. Mech. Techn. Phys., Russia* 36, 347-353 (1995).	Ignition Coal Particles Shock Tube Numerical Analysis
(77670)	Hot Surface, Ignition Temperatures, Dolomite, Limestone Admixture Effects	Coal Dust
(77671)	Ignition Temperatures, Salt Catalysis, Metal Ionization Potential and H_2O Effects	Coal
(77697)	Impact Ignition, Mechanisms, Review	Energetic Materials
(77711)	Ignition, Turbulent Boundary Layer Oxidizing Flow	PMMA
77729.	Kreutz, T.G., and C.K. Law, "Ignition in Nonpremixed Counterflowing Hydrogen versus Heated Air: Computational Study with Skeletal and Reduced Chemistry," *Combust. Flame* 114, 436-456 (1998).	Ignition Counterflow H_2/Hot Air Reduced Scheme Kinetic Modeling
77730.	Sheu, W.J., and M.C. Lin, "Ignition of Nonpremixed Wall-Bounded Boundary-Layer Flows," *Combust. Sci. Technol.* 122, 231-255 (1997).	Ignition Hot Wedge Porous Wall Fuel Ignition Modeling

77731. Mendez, F., and C. Trevino, "Ignition in a Vertical Wall in Contact with a Combustible Gas: Catalytic Reactions in One Surface of the Plate, "*Combust. Theory Modeling* 1, 167-182 (1997).

Ignition
Propagation
Catalytic
Vertical Wall
Combustible Gases
Model

77732. Veser, G., J. Frauhammer, L.D. Schmidt and G. Eigenberger, "Catalytic Ignition during Methane Oxidation on Platinum: Experiments and Modeling," pp. 273-284 in *Dynamics of Surfaces and Reaction Kinetics in Heterogeneous Catalysis*, G.F. Froment and K.C. Waugh, eds., Proceedings of the International Symposium Held in Antwerp, Belgium, September 1997, 53 Papers, 597 pp., Elsevier, Amsterdam, The Netherlands (1997).

Ignition
Temperatures
Catalytic
CH_4/Air/Pt
Behavior

(77703) ADN, $NH_4N(NO_2)_2$, Gaseous Species, Probe Sampling, Mass Analysis

Laser Ignition

11. COMBUSTION THEORY/PROPAGATION/STABILIZATION

77733. De Goey, L.P.H., and J.H.M.T.T. Boonkkamp, "A Mass-Based Definition of Flame Stretch for Flames with Finite Thickness," *Combust. Sci. Technol.* 122, 399-405 (1997).

Flame Stretch
Definition
Flame Front
Thickness
Effects

77734. Blouquin, R., G. Joulin and Y. Merhari, "Combustion Regimes of Particle-Laden Gaseous Flames: Influences of Radiation, Molecular Transports, Kinetic-Quenching, Stoichiometry," *Combust. Theory Modeling* 1, 217-242 (1997).

Combustion Theory
Inert Solid
Seeding
Flame Structure
Modeling

77735. Libby, P.A., and M.D. Smooke, "The Computation of Flames in Stagnation Flows," *Combust. Sci. Technol.* 127, 197-211 (1997).

Combustion Theory
Opposed/
Impinging Jets
Flow Structure
Formulations

77736. Cor, J.J., and M.C. Branch, "Studies of Counterflow Diffusion Flames at Low Pressures," *Combust. Sci. Technol.* 127, 71-88 (1997).

Counterflow
Low Pressure
Diffusion Flames
$CH_4/N_2O,O_2$
CO/N_2O
T,Species Profiles
Kinetic Modeling

77737. Bedir, H., J.S. T'ien and H.S. Lee, "Comparison of Different Radiation Treatments for a One-Dimensional Diffusion Flame," *Combust. Theory Modeling* 1, 395-404 (1997).

Diffusion Flames
Radiative
Heat Transfer
Model
Comparisons

77738. Abramovich, G.N., "Initial Section of Gas Nozzle-Burner Flame with Unsymmetrical Boundary Conditions," *Russ. Aeronaut.* 38(3), 37-41 (1995).

Diffusion Flame Theory
Unsymmetrical Flows
CH_4,C_3H_8,H_2/Air

77739. Pitsch, H., and N. Peters, "A Consistent Flamelet Formulation for Nonpremixed Combustion Considering Differential Diffusion Effects," *Combust. Flame* 114, 26-40 (1998).

Diffusion Flames
Differential Diffusion Model
H_2/Air
n-C_7H_{16}/Air

77740. Echekki, T., and J.H. Chen, "Structure and Propagation of Methanol/Air Triple Flames," *Combust. Flame* 114, 231-245 (1998).

CH_3OH/Air
Triple Flames
Structure
Differential Diffusional Effects
DNS Analysis

77741. Clavin, P., and G. Joulin, "High Frequency Response of Premixed Flames to Weak Stretch and Curvature: A Variable-Density Analysis," *Combust. Theory Modeling* 1, 429-446 (1997).

Premixed Flames
Velocity/Front Fluctuation Effects
Burning Speeds

77742. Chen, J.-Y., "Stochastic Modeling of Partially Stirred Reactors," *Combust. Sci. Technol.* 122, 63-94 (1997).

H_2/Air Combustion
Partially Stirred Reactor
Unmixedness
NO Formation
Effects,Modeling

77743. Mao, F., and R.B. Barat, "Experimental and Modeling Studies of Staged Combustion Using a Reactor Engineering Approach," *Chem. Eng. Commun.* 145, 1-21 (1996).

Combustion Studies
2-Stage Flow Reactor
Probe Sampling Method

77744. Najm, H.N., P.H. Paul, C.J. Mueller and P.S. Wyckoff, "On the Adequacy of Certain Experimental Observables as Measurements of Flame Burning Rate," *Combust. Flame* 113, 312-332 (1998).

Combustion
Heat Release
HCO/PLIF Correlation
CH_4/Air/N_2
Radical Emission
Alternates
Adequacies

77745.	Garbey, M., and D. Tromeur-Dervout, "Massively Parallel Computation of Stiff Propagating Combustion Fronts," *Combust. Theory Modeling* 1, 271-294 (1997).	Combustion Theory Propagation Stiff Integration Methodology
77746.	Ashurst, W.T., "Darrieus-Landau Instability, Growing Cycloids and Expanding Flame Acceleration," *Combust. Theory Modeling* 1, 405-428 (1997).	Expanding Premixed Flames Propagation Acceleration Modeling
77747.	Bychkov, V.V., A.I. Kleev and M.A. Liberman, "A Thin Front Model Applied to Flame Propagation in Tubes," *Combust. Flame* 113, 470-472 (1998).	Propagation Curved Flame Velocities Tubes Model
(77724)	Alkane,-ene, Low Temperature Combustion, Auto-ignition, Kinetic Mechanisms, Review	Cool Flames
77748.	Maunuksela, J., M. Myllys, O.-P. Kahkonen, J. Timonen, N. Provatas, M.J. Alava and T. Ala-Nissila, "Kinetic Roughening in Slow Combustion of Paper," *Phys. Rev. Lett.* 79, 1515-1518 (1997).	Paper Combustion Flame Front Propagation Kinetic Formulations
77749.	Brailovsky, I., and G.I. Sivashinsky, "On Stabilization and Blowoff of Inverted Spherical Flames," *Combust. Sci. Technol.* 122, 95-111 (1997).	Spherical Flames Stabilization Theory
77750.	Vedarajan, T.G., and J. Buckmaster, "Edge-Flames in Homogeneous Mixtures," *Combust. Flame* 114, 267-273 (1998).	Edge Flames Theory Stabilities
77751.	Kortsarts, Y., I. Brailovsky, S. Gutman and G.I. Sivashinsky, "On the Stability of Stretched Flames," *Combust. Theory Modeling* 1, 143-156 (1997).	Stretched Flames Stability Flow Induced Modeling
77752.	Kortsarts, Y., I. Brailovsky and G.I. Sivashinsky, "On Hydrodynamic Instability of Stretched Flames," *Combust. Sci. Technol.* 123, 207-225 (1997).	Counterflow Flames Instabilities Stretch Effects Modeling
77753.	Ju, Y., H. Guo, K. Maruta and T. Niioka, "Flame Bifurcations and Flammable Regions of Radiative Counterflow Premixed Flames with General Lewis Numbers," *Combust. Flame* 113, 603-614 (1998).	Stability Counterflow Premixed Radiative Flames Lewis Number Effects

(77664) Active Control, Dump Combustor, Hysterisis Method — Stabilization

12. TURBULENCE

(See also Section 14 for Turbulent Flame Velocities)

77754. Gouldin, F.C., "Analysis of Certain Algebraic Closure Models for Premixed Turbulent Combustion," pp. 433-459 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).
Turbulent Combustion
3 Closure Models
Assessments
Premixed Flames

77755. Denet, B., "A Lagrangian Method to Simulate Turbulent Flames with Reconnections," *Combust. Sci. Technol.* 123, 247-260 (1997).
Turbulent Flames
Lagrangian Formulation
Fractal Dimension

77756. McDonough, J.M., "On Intrinsic Errors in Turbulence Models Based on Reynolds-Averaged Navier-Stokes Equations," *Fluid Mech. Res.* 22(2), 27-55 (1995).
Turbulent Modeling
Reynolds Averaging
Intrinsic Errors
Analysis

77757. Swaminathan, N., and R.W. Bilger, "Direct Numerical Simulation of Turbulent Nonpremixed Hydrocarbon Reaction Zones Using a Two-Step Reduced Mechanism," *Combust. Sci. Technol.* 127, 167-196 (1997).
Turbulent Diffusion Flames
DNS Modeling
2-Step Reduced Kinetic Scheme

77758. Sabel'nikov, V., B. Deshaies and L.F.F. Da Silva, "Revisited Flamelet Model for Nonpremixed Combustion in Supersonic Turbulent Flows," *Combust. Flame* 114, 577-584 (1998).
Turbulent
Supersonic Flows
Stretched Flamelet Model

77759. Dyne, B.R., and J.C. Heinrich, "Finite Element Analysis of the Scramaccelerator with Hydrogen/Oxygen Combustion," Presented Originally as AIAA Paper 93-0745 at the *31st AIAA Aerospace Sciences Meeting and Exhibit*, Held in Reno NV, January 1993, *J. Propulsion Power* 12, 336-340 (1996).
Supersonic
Scramaccelerator
H_2/O_2 Thruster
Kinetic/Transport Modeling

77760. Lin, C.-Y., "Effects of Da and Re on Premixed Flame Speed," *Chem. Eng. Commun.* 155, 65-72 (1996).
Turbulent Premixed
Flame Speeds
Re,Da Dependences

77761.	Sabel'nikov, V.A., C. Corvellec and P. Bruel, "Analysis of the Influence of Cold Front Quenching on the Turbulent Burning Velocity Associated with an Eddy-Break-Up Model," *Combust. Flame* 113, 492-497 (1998).	Turbulent Eddy Break-up Model Burning Velocities Quenching Effects
77762.	Johnson, M.R., L.W. Kostiuk and R.K. Cheng, "A Ring Stabilizer for Lean Premixed Turbulent Flames," *Combust. Flame* 114, 594-596 (1998).	Turbulent Lean Flames Ring Stabilizer
77763.	Choi, C.R., and K.Y. Huh, "Development of a Coherent Flamelet Model for a Spark Ignited Turbulent Premixed Flame in a Closed Vessel," *Combust. Flame* 114, 336-348 (1998).	Turbulent Flamelet Model Propagation Well Quenching Closed Vessel Burning Velocities
77764.	Furukawa, J., T. Hirano and F.A. Williams, "Burning Velocities of Flamelets in a Turbulent Premixed Flame," *Combust. Flame* 113, 487-491 (1998).	Turbulent Premixed C_3H_8/Air Flamelet Burning Velocities Probe, LDV Measurements
77765.	Bielert, U., and M. Sichel, "Numerical Simulation of Premixed Combustion Processes in Closed Tubes," *Combust. Flame* 114, 397-419 (1998).	Turbulent Closed Tube Combustion Propagation CH_4/Air C_2H_4/O_2 Model
77766.	Zimberg, M.J., S.H. Frankel, J.P. Gore and Y.R. Sivathanu, "A Study of Coupled Turbulent Mixing, Soot Chemistry and Radiation Effects Using the Linear Eddy Model," *Combust. Flame* 113, 454-469 (1998).	Turbulent C_2H_2/Air Soot/Radiation Interactions Linear Eddy Model
77767.	Goldin, G.M., and S. Menon, "A Comparison of Scalar PDF Turbulent Combustion Models," *Combust. Flame* 113, 442-453 (1998).	Turbulent Combustion CH_4, H_2 Jets Scalar PDFs Model Comparisons
(78068)	Turbulent, Temperature, H_2 Density CARS Measurements	H_2 Jet
77768.	Lee, T.-W., and A. Mitrovic, "Structure of Lean Turbulent Partially-Premixed Flames Stabilized in a Coaxial Jet Flame Burner," *Combust. Sci. Technol.* 127, 231-249 (1997).	Turbulent Coaxial Jet Lean Premixed Flames Rayleigh T PDFs Stability

(77904) Turbulent 2-Phase, Particle Sizes, Densities, Tomographic Laser Diffraction Method — Coaxial Jet

(77879) Turbulent, NO_x Formation, Model — CH_4 ,CO/H_2 H_2 Jet Flames

77769. Kelman, J.B., and A.R. Masri, "Simultaneous Imaging of Temperature and OH Number Density in Turbulent Diffusion Flames," *Combust. Sci. Technol.* 122, 1-32 (1997). — Turbulent CH_4 ,CH_3OH,C_2H_5OH Diffusion Flames OH,LIF T,Rayleigh Imaging

77770. Dally, B.B., A.R. Masri, R.S. Barlow and G.J. Fiechtner, "Instantaneous and Mean Compositional Structure of Bluff-Body Stabilized Nonpremixed Flames," *Combust. Flame* 114, 119-148 (1998). — Turbulent Diffusion Flames CH_4/H_2 ;CO/H_2 CH_3OH Raman/LIF/ Rayleigh Species Profiles

77771. Kuperjans, S., and I.M. Kennedy, "Measurements of NO_x in Turbulent Diffusion Flames with High Speed Co-Flow Air," pp. 69-85 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997). — Turbulent C_2H_4 ,C_3H_8 ,H_2 Diffusion Flames NO,NO_2 ,Soot Radiation Measurements

77772. Karpov, V.P., and A.N. Lipatnikov, "An Effect of Molecular Thermal Conductivity and Diffusion on Premixed Combustion," *Dokl. Phys. Chem.* 341, 83-85 (1995). — Turbulent Burning Velocities $CH_4/H_2/O_2/N_2$ $H_2/O_2/N_2$ Spherical Flames Calculations Data Comparisons

13. DETONATIONS/EXPLOSIONS

77773. Cooper, P.W., and S.R. Kurowski, *"Introduction to the Technology of Explosives,"* 8 Chapters, 204 pp., Wiley-VCH, Inc., New York (1996). — Explosives Chemistry Initiation Combustion Monograph

77774. Li, T., "Rigorous Asymptotic Stability of a Chapman-Jouguet Detonation Wave in the Limit of Small Resolved Heat Release," *Combust.Theory Modeling* 1, 259-270 (1997). — Detonation Theory Wave Stability

77775. Short, M., "A Parabolic Linear Evolution Equation for Cellular Detonation Instability," *Combust. Theory Modeling* 1, 313-346 (1997).

Cellular Detonations Instabilities Front Curvature Role Modeling

(78140) MPD, Diatomics Recombination Heating, Model

Thermal Explosion

77776. Zhang, F., P.A. Thibault and S.B. Murray, "Transition from Deflagration to Detonation in an End Multiphase Slug," *Combust. Flame* 114, 13-25 (1998).

Deflagration/ Detonation Al Dust/ C_2H_2/Air End Wall Pressures

(77929) High Pressure Detonation Regime, Raman Spectra

CH_3NO_2, CD_3NO_2 $C_2H_5NO_2$

77777. Lindstedt, R.P., and V. Sakthitharan, "Time Resolved Velocity and Turbulence Measurements in Turbulent Gaseous Explosions," *Combust. Flame* 114, 469-483 (1998).

Explosions Turbulent CH_4/Air Obstacle Initiation LDA Velocities

(77707) RDX, $(CH_2NNO_2)_3$, Primary Flame Kinetic Modeling

Deflagration Velocities

77778. Thaker, A.A., and H.K. Chelliah, "Numerical Prediction of Oblique Detonation Wave Structures Using Detailed and Reduced Reaction Mechanisms," *Combust. Theory Modeling* 1, 347-376 (1997).

Detonations Oblique Wave Structure H_2/Air Reduced Kinetic Schemes

77779. Dautov, N.G., and A.M. Starik, "Effect of Excitation of Molecular Vibrations on the Dynamics of Combustion of an H_2/O_2 Mixture Behind a Detonation Shockwave," *J. Appl. Mech. Techn. Phys., Russia* 36, 818-825 (1995).

Detonations H_2/O_2 Vibrational Energy Effects Acceleration

14. FLOW PHENOMENA/VELOCITIES/DIFFUSION

(See also Section 12 for Turbulent Flowfields)

77780. Raffel, M., C.E. Willert and J. Kompenhans, *"Particle Image Velocimetry: A Practical Guide,"* 253 pp., Springer-Verlag, Berlin, Germany (1998).

PIV Technique Monograph

77781. Dunn-Rankin, D., and F. Weinberg, "Location of the Schlieren Image in Premixed Flames: Axially Symmetrical Refractive Index Fields," *Combust. Flame* 113, 303-311 (1998).

Flame Shape
Visualization
Schlieren Image
Analytical Solutions
R.I. Fields

(77667) Swirling Coal Flame, Species Transport and Profiles, Temperatures, Modeling

Flowfield

(77677) Particle Dispersion, Turbulent Fluid, Modeling

2-Phase Flowfield

(77680) Spray Flames, Kerosene, Sizes, Transport

Droplet Velocities

77782. Cetegen, B.M., "Measurements of Instantaneous Velocity Field of a Non-Reacting Pulsating Buoyant Plume by Particle Image Velocimetry," *Combust. Sci. Technol.* 123, 377-387 (1997).

Buoyant Plumes
Pulsating
He/Air
Velocity Flowfield
PIV

(77747) Propagation, Tubes, Model

Curved Flame
Velocities

(77665) Flowfield, Curved Wall Jet Burner, Blow-off, Flame Length, Stabilization

LDV

(77777) Velocities, Turbulent Explosive CH_4/Air, Obstacle Initiated

LDA

77783. Mallens, R.M.M., B.O. Loijenga, L.P.H. De Goey and P.J.M. Sonnemans, "Numerical and Experimental Study of Lean M- and V-Shaped Flames," *Combust. Sci. Technol.* 122, 331-344 (1997).

V,M-Shaped
CH_4/Air
Lean Flames
Flowfields
LDV
Modeling

77784. Grandmaison, E.W., I. Yimer, H.A. Becker and A. Sobiesiak, "The Strong Jet/Weak Jet Problem and Aerodynamic Modeling of the Canadian Gas Research Institute Burner," *Combust. Flame* 114, 381-396 (1998).

Weak Fuel Jet
Strong Air Jet
Interactions
Flowfield
Low NO_x Burner

77785. Lee, B.J., M.S. Cha and S.H. Chung, "Characteristics of Laminar Lifted Flames in a Partially Premixed Jet," *Combust. Sci. Technol.* 127, 55-70 (1997).

Premixed Jet
Flame Lengths
Blow-off
Velocities
C_3H_8,C_4H_{10}/Air
Correlations

77786.	Bourehla, A., and F. Baillot, "Appearance and Stability of a Laminar Conical Premixed Flame Subjected to an Acoustic Perturbation," *Combust. Flame* 114, 303-318 (1998).	Conical Flame CH_4/Air Acoustically Induced Upstream Flow Fluctuations LDV,Stabilities
77787.	Ishizuka, S., T. Murakami, T. Hamasaki, K. Koumura and R. Hasegawa, "Flame Speeds in Combustible Vortex Rings," *Combust. Flame* 113, 542-553 (1998).	Flame Speeds CH_4/Air Vortex Rings Measurements
77788.	Stone, R., A. Clarke and P. Beckwith, "Correlations for the Laminar-Burning Velocity of Methane/Diluent/Air Mixtures Obtained in Free-Fall Experiments," *Combust. Flame* 114, 546-555 (1998).	Burning Velocities CH_4/Air/CO_2,N_2 Microgravity P,T Correlations
(78082)	Rich, Premixed CH_4/Air, Asymptotic Analysis, Flame Structure, Reduced Kinetics	Burning Velocities
(77814)	CH_4/Air/$CHCl_3$, CH_2Cl_2, Inhibition Effects, Kinetic Modeling	Burning Velocities
77789.	Saso, Y., D.L. Zhu, H. Wang, C.K. Law and N. Saito, "Laminar Burning Velocities of Trifluoromethane/Methane Mixtures: Experiment and Numerical Simulation," *Combust. Flame* 114, 457-468 (1998).	Burning Velocities CH_4/CHF_3/O_2 Inhibition Kinetic Modeling Comparisons
(77764)	Flamelet Burning Velocities, Turbulent Premixed C_3H_8/Air	LDV
(77685)	C_7H_{16}/$C_{16}H_{34}$ Reduced Gravity Droplet Combustion	Liquid Species Diffusion Coefficients
(78016)	Diffusion Coefficient Measurement, He/Cs Pulsed Hollow Cathode Discharge	He(2^3S)/Cs
(78129)	Diffusion Constant, DFWM Monitor	NaH/H_2

15. IONIZATION

(See also Section 26 for Ion Spectroscopy, Section 27 for Penning Ionization, Section 40 for Dynamics of Ion-Molecule Reactions, Section 42 for MPI, Section 44 for Ionic Structures and Section 46 for Thermochemical Values)

77790. Axford, S.D.T., J.M. Goodings and A.N. Hayhurst, "Mass Spectrometric Sampling of Ions from Flames at Atmospheric Pressure: The Effects of Applied Electric Fields and the Variation of Electric Potential in a Flame," *Combust. Flame* 114, 294-302 (1998).

Flame Ions
H_2/O_2/Cs/Inert
Mass Spectrometric Sampling Nozzle
Electric Field Effects

(77719) Role, NH_3/O_2/Pt Catalytic Oxidation — Charged Particles

(77720) Role, SO_2/Air/Fe_2O_3, Catalytic Oxidation — Charged Particles

77791. Tennyson, J., "Theory of Low Energy Electron-Molecule Dissociative Recombination," *Comments At. Mol. Phys.* 32, 209-218 (1996).

$AB^+ + e^-$
Dissociative Recombination
Theory
Current Status

77792. Farrar, J.M., "Ion Reaction Dynamics," *Ann. Rev. Phys. Chem.* 46, 525-554 (1995).

Ion/Molecule Reaction Dynamics
$O^- + D_2$, HF, H_2O
$C_2H_2^+$, NH_3^+
Review

(78061) Atomic Analysis, Detection Limits, Methods, Review — Laser Induced Ionization

(78062) Laser Ablation, Lanthanides, Mass Analysis Method — M^+, MO^+ Plumes

77793. Sheng, L., F. Qi, H. Gao, Y. Zhang, S. Yu and W.-K. Li, "Experimental and Theoretical Study of the Photoionization and Dissociative Photoionizations of Dichlorodifluoromethane," *Int. J. Mass Spectrom. Ion Process.* 161, 151-159 (1997).

CCl_2F_2
Photoionization
Product Ions
Channels

77794. Jarvis, G.K., C.A. Mayhew, L. Singleton and S.M. Spyrou, "An Investigation of Electron Attachment to $CHCl_2F$, $CHClF_2$ and CHF_3 Using an Electron-Swarm Mass Spectrometric Technique," *Int. J. Mass Spectrom. Ion Process.* 164, 207-223 (1997).

$CHCl_2F + e^-$
$CHClF_2$, $CHF_3 + e^-$
Attachment
Rate Constants

77795. Tsuji, M., M. Nakamura, Y. Nishimura and H. Obase, "Nascent Rovibrational Distributions of $CO(d^3\Delta_i, e^3\Sigma^-, a'\ ^3\Sigma^+)$ Produced in the Dissociative Recombination of CO_2^+ with Electrons," *J. Chem. Phys.* 108, 8031-8038 (1998).

$CO_2^+ + e^-$
Dissociative Recombination
CO(d,e,a′),v,J
Product Formation
Rate Constants

77796. Skrzypkowski, M.P., T. Gougousi, R. Johnsen and M.F. Golde, "Measurement of the Absolute Yield of $CO(a^3\Pi) + O$ Products in the Dissociative Recombination of CO_2^+ Ions with Electrons," *J. Chem. Phys.* 108, 8400-8407 (1998).

$CO_2^+ + e^-$
Dissociative Recombination
CO(a) Product Yield
$CO(a) + CO_2$
Quenching
Rate Constant

77797.	Qian, J., R.J. Green and S.L. Anderson, "A Mode-Selective Differential Scattering Study of the $C_2H_2^+$ + Methanol Reaction: Influence of Collision Intermediates, Collision Times and Transition States," *J. Chem. Phys.* 108, 7173-7184 (1998).	$C_2H_2^+ + CD_3OD$ $C_2H_2^+ + CD_3OH, CH_3OD$ Cross Sections Branching Ratios Energy Dependences
77798.	Chen, Y.-J., S. Stimson, P.T. Fenn, C.Y. Ng, W.-K. Li and N.L. Ma, "A Study of the Dissociation of $CH_3CH_2SH^+$ by Collisional Activation: Evidence of Nonstatistical Behavior," *J. Chem. Phys.* 108, 8020-8028 (1998).	$C_2H_5SH^+ + Ar$ Dissociation Product Ion Cross Sections $C_2H_5SH + h\nu$ 1-Photon Ionization Comparisons
77799.	Rebrion-Rowe, C., L. Lehfaoui, B.R. Rowe and J.B.A. Mitchell, "The Dissociative Recombination of Hydrocarbon Ions. II. Alkene and Alkyne Derived Species," *J. Chem. Phys.* 108, 7185-7189 (1998).	$C_4H_5^+, C_4H_{11}^+ + e^-$ $C_5H_9^+, C_6H_4^+ + e^-$ $C_6H_5^+, C_8H_7^+ + e^-$ Dissociative Recombination Rate Constants
(77911)	355 nm Induced Thermionic Emission, Delayed Electron Efficiency	C_{60}
77800.	Laskin, J., C. Weickhardt and C. Lifshitz, "Time-Resolved Kinetic Energy Releases for $C_{60}^+ \rightarrow C_{58}^+ + C_2$," *Int. J. Mass Spectrom. Ion Process.* 161, L7-L11 (1997).	C_{60}^+ C_2 Elimination Measurements Transition State Dynamics
(78149)	UV/Visible Fragmentation Patterns, 24 PAHs	$C_{60}^+ + h\nu$ $PAH^+ + h\nu$
77801.	Griffin, J.B., and P.B. Armentrout, "Guided Ion Beam Studies of the Reactions of Cr_n^+ (n=1-18) with CO_2: Chromium Cluster Oxide Bond Energies," *J. Chem. Phys.* 108, 8075-8083 (1998).	$Cr_n^+ + CO_2$ n=1-18 Product Ions Cross Sections $D(Cr_n^+O)$
77802.	Griffin, J.B., and P.B. Armentrout, " Guided Ion Beam Studies of the Reactions of Cr_n^+ (n=2-18) with O_2: Chromium Cluster Oxide and Dioxide Bond Energies," *J. Chem. Phys.* 108, 8062-8074 (1998).	$Cr_n^+ + O_2$ n=2-18 Product Ions Cross Sections $D(Cr_mO_2^+)$
77803.	Blanchet, V., M.A. Bouchene and B. Girard, "Temporal Coherent Control in the Photoionization of Cs_2: Theory and Experiment," *J. Chem. Phys.* 108, 4862-4876 (1998).	Photoionization $Cs_2(B)$ Laser Control fs 2-Pulse Method
(77717)	Role, CO/O_2/Pt Catalytic Oxidation, ps Laser Induced	Nonthermal Substrate Electrons

(77866) CH_2Cl_2/Air, N_2 Destructive Incineration, Discharge Methods, Products | e-Beam Method

77804. Cipollini, R., M.E. Crestoni and S. Fornarini, "Positive Ion Chemistry of Elemental Fluorine," *J. Am. Chem. Soc.* 119, 9499-9503 (1997). | $F_2^+ + M$ 20 Ion/Molecule Reactions Rate Constants Products

77805. Schroder, D., H. Schwarz, D.E. Clemmer, Y. Chen, P.B. Armentrout, V.I. Baranov and D.K. Bohme, "Activation of Hydrogen and Methane by Thermalized FeO^+ in the Gas Phase as Studied by Multiple Mass Spectrometric Techniques," *Int. J. Mass Spectrom. Ion Process.* 161, 175-191 (1997). | $FeO^+ + CH_4$ $FeO^+ + H_2$ Rate Constants Product Ions Dynamics

77806. Grimbert, D., V. Sidis and V. Cobut, "Effects of Complex Formation on Low Energy $H^+ + O_2(X^3\Sigma_g^-, v=0) \rightarrow H + O_2^+(X^2\Pi_g, v'')$ Charge Transfer," *J. Chem. Phys.* 108, 6331-6341 (1998). | $H^+ + O_2$ Charge Exchange $O_2^+(v)$ Product Cross Sections Calculations

(78262) IR fs Laser Pulse Reaction Control, D^+, D Product Branching Method | $HD^+ + h\nu$

(78268) Energy Levels, Near Dissociation Limit Spectroscopy, Theory/Experiment, Review | H_2^+, HD^+, D_2^+

(78177) 17 eV Energy, OH, OD(A,v,J) Product Distributions | $H_2O, D_2O + e^-$

(77888) Corona Discharge Method, Electrode Material Effects | NO_x Control

(77887) Discharge Method, Major Channels, Kinetics | NO, NO_2, SO_2 Emissions Control

(77889) Back Corona Discharge Method | NO_2/N_2 Dissociation

77807. Oddone, S., J.W. Sheldon, K.A. Hardy and J.R. Peterson, "Dissociative Recombination of the $A^2\Pi_u$ and the $X^2\Sigma_g$ States of N_2^+ in a Glow Discharge," *Phys. Rev. A: At. Mol. Opt. Phys.* 56, 4737-4741 (1997). | $N_2^+(A,X) + e^-$ Dissociative Recombination Product Branching Ratios

77808. Mwakapumba, J., and K.M. Ervin, "Reactivity of Niobium Cluster Anions with Nitrogen and Carbon Monoxide," *Int. J. Mass Spectrom. Ion Process.* 161, 161-174 (1997). | $Nb_n^- + CO, N_2$ Rate Constants $n=2$-7 Absorption/ Fragmentation

77809. Berg, C., M. Beyer, U. Achatz, S. Joos, G. Niedner-Schatteburg and V.E. Bondybey, "Effect of Charge Upon Metal Cluster Chemistry: Reactions of Nb_n and Rh_n Anions and Cations with Benzene," *J. Chem. Phys.* 108, 5398-5403 (1998). | $Nb_n^- + C_6H_6$ $Rh_n^- + C_6H_6$ Relative Rate Constants $n=3$-28

(78158) Photodetachment Spectrum Calculations — $OHCl^- + h\nu$

(78289) P.E. Curves, Low-lying States, Photodissociation Processes — O_3^-

(78051) Emission Branching Ratio Measurement — $P^+(^5S_2\text{-}^3P_{2,1})$

77810. Sparrapan, R., M.A. Mendes, I.P.P. Ferreira, M.N. Eberlin, C. Santos and J.C. Nogueira, "Gas Phase Chemistry of the Sulfur Hexafluoride Fragment Ions SF_n^+ (n=0-5) and SF_n^{2+} (n=2,4): Ab Initio Thermochemistry of Novel Reactions of S^+ and SF^+," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5189-5195 (1998).
$SF_n^+ + CO, CO_2, O_2$
$SF_n^+ + H_2O, N_2O$
n=0-5
Product Channels
Measurements
Calculations

77811. Lovejoy, E.R., and R.R. Wilson, "Kinetic Studies of Negative Ion Reactions in a Quadrupole Ion Trap: Absolute Rate Coefficients and Ion Energies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2309-2315 (1998).
$SF_6^- + HCl, HNO_3, SO_2$
$NO_3^- + HNO_3 + He$
Rate Constants
Branching Ratios

77812. Ye, S., "Theoretical Study of the Dehydrogenation Reaction of Water by Sc^+," *J. Mol. Struct.* 417, 157-162 (1997).
$Sc^+ + H_2O$
Channels
Sc^+O Product
Reaction Dynamics
Energies

77813. Xu, J., M.T. Rodgers, J.B. Griffin and P.B. Armentrout, "Guided Ion Beam Studies of the Reactions of V_n^+ (n=2-17) with O_2: Bond Energies and Dissociation Pathways," *J. Chem. Phys.* 108, 9339-9350 (1998).
$V_n^+ + O_2$, n=2-17
Channels
Energy Dependences
$D(V_n^+\text{-}O)$, n=2-15

16. INHIBITION/ADDITIVES

(See also Section 21 for Combustion Emission Control Additives)

(77789) Inhibition, CH_4/O_2 Burning Velocity Effects, Kinetic Modeling Comparisons — CHF_3

77814. Leylegian, J.C., D.L. Zhu, C.K. Law and H. Wang, "Experiments and Numerical Simulation on the Laminar Flame Speeds of Dichloromethane and Trichloromethane," *Combust. Flame* 114, 285-293 (1998).
Inhibition
$CH_4/Air/CH_2Cl_2$
$CH_4/Air/CHCl_3$
Flame Speeds
Kinetic Modeling

77815. Sanogo, O., J.-L. Delfau, R. Akrich and C. Vovelle, "Experimental and Modeling Study of the Effect of CF_3CHFCF_3 on the Chemical Structure of a Methane/Oxygen/Argon Flame," *Combust. Sci. Technol.* 122, 33-62 (1997).
Inhibition
$CH_4/O_2/Ar$
C_3HF_7 Effects
Beam Sampling
Mass Analysis
Flame Structure

77816. Hynes, R.G., J.C. Mackie and A.R. Masri, "Inhibition of Premixed Hydrogen/Air Flames by 2-*H* Heptafluoropropane," *Combust. Flame* 113, 554-565 (1998).
Inhibition
$H_2/Air/C_3HF_7$
Species Profiles
Kinetic Model

(78141) $CF_3Br + h\nu$, IR Dissociation, Isotopic Enrichment, Enhancement Effects — NO Effects

(77670) Hot Surface Ignition Temperatures, Admixture Effects — Coal/Dolomite, Coal/Limestone

(77671) Coal Ignition Temperatures, Metal Ionization Potential and H_2O Effects — Salt Catalysis

(78253) Additive Effects on n-C_7H_{16}/O_2, Jet Stirred Reactor, Fuel Knocking Tendencies — MTBE,ETBE

(78086) Burnt Gases, CO, NO Kinetics — HCl Effects

77817. Trees, D., and K. Seshadri, "Experimental Studies of Flame Extinction by Sodium Bicarbonate ($NaHCO_3$) Powder," *Combust. Sci. Technol.* 122, 215-230 (1997).

Extinction
Hydrocarbon Flames
$NaHCO_3$ Powder Effectiveness

(78075) Additives, $H_2/O_2/Ar$, $CH_3PO(OCH_3)_2$ and $(CH_3)_3PO_4$, Products, Mass Spectra — Organophosphorus

17. CORROSION/EROSION/DEPOSITION

(See also Section 22 for Diamond Formation Deposition)

77818. Perrin, J., O. Leroy and M.C. Bordage, "Cross Sections, Rate Constants, and Transport Coefficients in Silane Plasma Chemistry," *Contrib. Plasma Phys.* 36, 3-49 (1996).

Deposition
Si Films
SiH_4
Low Pressure Glow Discharges
Reaction Scheme
Rate Constants
Review

77819. Aleksandrov, S.E., M.L. Khitchman, F.F. Grekov and V.S. Ivanov, "Remote Plasma Enhanced Chemical Vapor Deposition of Silicon Nitride Films in the System $SiH_4/N_2/NF_3$," *Russ. J. Appl. Chem.* 69, 1118-1125 (1996).

CVD
Si_3N_4
Films
$SiH_4/N_2/NF_3$
Discharge

18. GAS/SURFACE INTERACTIONS/BOUNDARY LAYER COMBUSTION

(See also Section 7 for Catalytic Combustion, Section 17 for Deposition and Section 22 for Particle Formation and Deposition)

77820. Sirignano, W.A., and D.N. Schiller, "Mechanisms of Flame Spread Across Condensed Phase Fuels," pp. 353-407 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).

Flame Spread
Solid Fuels
Liquid Pools
Mechanisms
Review

77821.	Mercer, G.N., and R.O. Weber, "Combustion Waves in Two Dimensions and Their One-Dimensional Approximation," *Combust. Theory Modeling* 1, 157-165 (1997).	Fuel Layer Propagation 2-D Combustion Wave Model
77822.	Carrier, G.F., F.E. Fendell and S.F. Fink IV, "Air Dilution, under Calm Conditions of Spreading Dense Vapor from an Instantaneous Spill of Volatile Liquid," *Combust. Flame* 114, 178-191 (1998).	Fuel Spill Spread Vaporization Model
77823.	West, J., M. King, S. Bhattacharjee and R.A. Altenkirch, "Heat Transfer Pathways in Flame Spreading Over Thick Fuels as a Function of the Flame Spread Regime: Microgravity, Thermal and Kinetic," *Combust. Sci. Technol.* 127, 119-140 (1997).	Flame Spread Thick Fuels Opposed Flow Heat Transfer Structure
77824.	Burelbach, J.P., M. Epstein and M.G. Plys, "Initiation of Flame Spreading on Shallow Subflash Fuel Layers," *Combust. Flame* 114, 280-282 (1998).	Flame Spread Shallow Alkane Layers Measurements
77825.	Hoover, J.B., J.L. Bailey and P.A. Tatem, "An Improved Radiation Transport Submodel for the Consolidated Fire Growth and Smoke Transport (CFAST) Model," *Combust. Sci. Technol.* 127, 213-229 (1997).	Fire Model Radiative Heat Transfer Algorithm CFAST Code
(77712)	Burning Rates, Water Spray Extinction, CFD Model	PMMA Fires
(78077)	Tomography, Feasibility Assessments	Fire Plumes
77826.	Wichman, I.S., N. Lakkaraju and B. Ramadan, "The Structure of Quenched Triple Flames Near Cold Walls in Convective Flows," *Combust. Sci. Technol.* 127, 141-165 (1997).	Flame/Wall Quenching Triple Flame Tip Modeling
(77763)	Turbulent Flamelet Model, Propagation, Closed Vessel, Burning Velocities	Flame/Wall Quenching
(77731)	Catalytic Vertical Wall, Combustible Gases, Ignition, Propagation, Model	Gas/Wall Combustion
(77686)	Surface Spin Combustion, Cylindrical Metal Sample, Model	Gas/Surface Combustion
(77672)	Carbon Packed Bed, Stagnation Point Flow, Simulation	Gas/Solid Combustion
(77711)	PMMA Heating, Ignition, Turbulence Effects	Boundary Layer Flows
(77869)	CO, Organics, Emissions Control, Efficiencies	Porous Cellular Catalysts

(77842) I.C. Engine, Emissions Control, Unburnt Hydrocarbons, CO, NO_x — Porous Cellular Catalysts

77827. Traa, Y., M. Breuninger, B. Burger and J. Weitkamp, "Oscillation of NO_x Concentration in the Selective Catalytic Reduction of Nitrogen Oxides on Platinum-Containing Zeolite Catalysts," *Angew. Chem. Int. Ed. Engl.* 36, 2113-2114 (1997).

Kinetic
Oscillations
NO_x
C_3H_6/Pt/V
Zeolites
H_2O Effects

77828. Ciambelli, P., A. Di Benedetto, E. Garufi, R. Pirone and G. Russo, "Self-Sustained Isothermal Oscillations in N_2O Decomposition on Cu Over-Exchanged ZSM-5," pp. 175-184 in *Dynamics of Surfaces and Reaction Kinetics in Heterogeneous Catalysis*, G.F. Froment and K.C. Waugh, eds., Proceedings of the International Symposium Held in Antwerp, Belgium, September 1997, 53 Papers, 597 pp., Elsevier, Amsterdam, The Netherlands (1997).

Catalytic
Dissociation
N_2O/Cu Zeolite
Oscillations
O_2 Effects

77829. Li, K., X.F. Wang and H.C. Zeng, "Kinetics of N_2O Decomposition on a RuO_2/Al_2O_3 Catalyst," *Chem. Eng. Res. Design. Trans. Inst. Chem. Eng.* 75, 807-812 (1997).

Catalytic
Dissociation
$N_2O/RuO_2,Al_2O_3$
570-670 K
Kinetic Rates

77830. Hanson, D.R., "Reaction of $ClONO_2$ with H_2O and HCl in Sulfuric Acid and $HNO_3/H_2SO_4/H_2O$ Mixtures," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4794-4807 (1998).

Heterogeneous
$ClONO_2+H_2O/H_2SO_4$
$ClONO_2+HCl/H_2SO_4$
$ClONO_2+HNO_3/H_2SO_4$
Reaction
Probabilities

77831. Donsig, H.A., D. Herridge and J.C. Vickerman, "Static Secondary Ion Mass Spectrometry Studies of Reactions on Mimics of Polar Stratospheric Clouds. II: Low Temperature, Low Pressure Interactions of Cl_2 and Cl_2O with Solid Ice Films," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2302-2308 (1998).

Heterogeneous
Cl_2/Ice
Cl_2O/Ice
HOCl/Ice
Interactions

77832. Mochida, M., H. Akimoto, H. van den Bergh and M.J. Rossi, "Heterogeneous Kinetics of the Uptake of HOBr on Solid Alkali Metal Halides at Ambient Temperature," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4819-4828 (1998).

Heterogeneous
HOBr + NaCl(s)
HOBr + KBr(s)
Uptake
Coefficients
Br_2,BrCl
Product Yields

77833. Longfellow, C.A., T. Imamura, A.R. Ravishankara and D.R. Hanson, "HONO Solubility and Heterogeneous Reactivity on Sulfuric Acid Surfaces," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3323-3332 (1998).

Heterogeneous
$HONO/H_2SO_4(aq)$
Uptake
Coefficients

77834. Pallix, J.B., and R.A. Copeland, "Measurement of Catalytic Recombination Coefficients on Quartz Using Laser Induced Fluorescence," *J. Thermophys. Heat Transfer* 10, 224-233 (1996).

Heterogeneous
N,O/Quartz
Recombination
Coefficients
2-Photon LIF

77835. Schweitzer, F., P. Mirabel and C. George, "Multiphase Chemistry of N_2O_5, $ClNO_2$ and $BrNO_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3942-3952 (1998).

Heterogeneous
N_2O_5, $ClNO_2$
$BrNO_2$
Droplet Uptake
Coefficients
Salt Solution Effects

77836. Abbatt, J.P.D., and G.C.G. Waschewsky, "Heterogeneous Interactions of HOBr, HNO_3, O_3 and NO_2 with Deliquescent NaCl Aerosols at Room Temperature," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3719-3725 (1998).

Heterogeneous
NaCl Aerosols/M
M = HOBr, HNO_3,
NO_2, O_3
Uptake
Coefficients
pH Effects

19. ENGINES/EMISSIONS

(See also Section 10 for Ignition)

77837. Lee, D., and S. Hochgreb, "Rapid Compression Machines: Heat Transfer and Suppression of Corner Vortex," *Combust. Flame* 114, 531-545 (1998).

Rapid Compression
Machines
Piston Redesign
Corner Vortex
Suppression

77838. Bradley, D., and C. Morley, "Auto-ignition in Spark Ignition Engines," Chapter 7 in *Low Temperature Combustion and Autoignition*, M.J. Pilling, ed., 7 Chapters, 794 pp., *Comprehensive Chemical Kinetics* 35, 661-760 (1997).

I.C. Engines
Auto-ignition
Pressure Pulses
Predictive Models
Review

77839. Bell, S.R., and M. Gupta, "Extension of the Lean Operating Limit for Natural Gas Fueling of a Spark Ignited Engine Using Hydrogen Blending," *Combust. Sci. Technol.* 123, 23-48 (1997).

I.C. Engine
Lean Natural Gas/
H_2 Blends
Performance
Emissions

77840. Alasfour, F.N., "Butanol: A Single Cylinder Engine Study: Availability Analysis," *Appl. Thermal Eng.* 17, 537-549 (1997).

I.C. Engine
C_4H_9OH/Gasoline
Blends
Efficiencies

77841. Cartlidge, J., and J.K. Graham, "The Formation of Diheptylperoxide from *n*-Heptane in a Motored Engine," *Combust. Sci. Technol.* 127, 89-96 (1997).

I.C. Engine
n-C_7H_{16} Fuel
$(C_7H_{15})_2O_2$
Formation
Surface Role

77842. Antsiferov, V.N., M.Yu. Kalashnikova, A.M. Makarov and I.V. Filimonova, "Catalysts for Afterburning of Internal Combustion Engine Exhaust, Based on Highly Porous Cellular Materials," *Russ. J. Appl. Chem.* 70, 98-103 (1997).

I.C. Engine
UHC, CO,NO_x
Emissions Control
Porous
Cellular Catalysts

77843. Bi, H., and A.K. Agrawal, "Study of Auto-ignition of Natural Gas in Diesel Environments Using Computational Fluid Dynamics with Detailed Chemical Kinetics," *Combust. Flame* 113, 289-302 (1998).

Diesel Engine
Natural Gas
Auto-ignition
CFD/Kinetic
Modeling

77844. Kennedy, I.M., R. Milhacea, J. Kostka, M. Cramer, R. Pasek and D.P.Y. Chang, "NO_x and Hydrocarbon Emissions from a Diesel Engine Fueled on Digester Gas," *Combust. Sci. Technol.* 123, 63-82 (1997).

Diesel Engine
CH_4/CO_2 Synfuel
NO_x Emissions

77845. Cigizoglu, K.B., T. Ozaktas and F. Karaosmanoglu, "Used Sunflower Oil as an Alternative Fuel for Diesel Engines," *Energy Sources* 19, 559-566 (1997).

Diesel Engines
Sunflower Oil
Blended Fuel
Soot Emission
Effects

77846. Ergeneman, M., T. Ozaktas, K.B. Cigizoglu, F. Karaosmanoglu and E. Arslan, "Effect of Some Turkish Vegetable Oil/Diesel Fuel Blends on Exhaust Emissions," *Energy Sources* 19, 879-885 (1997).

Diesel Engines
Vegetable Oil
Blended Fuels
Emission Effects

77847. Litzinger, T.A., J.A. Pinson, D.O. Clark and D.L. Mitchell, "The Effect of Intake Charge Dilution with CO_2 on Diesel Soot Evolution," pp. 231-252 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).

Diesel Engines
Soot Formation
CO_2 EGR Effects
LII,Scattering
Sizes,Yields

77848. Higashi, M., S. Uchida, N. Suzuki and K.-i. Fujii, "Soot Elimination and NO_x and SO_x Reduction in Diesel Engine Exhaust by a Combination of Discharge Plasma and Oil Dynamics," *IEEE Trans. Plasma Sci.* 20, 1-12 (1992).

Diesel Engine
Soot,NO_x ,SO_2
Control
Downstream
Plasma Reactor
Method

77849. Park, D.S., J.U. Kim and E.S. Kim, "A Burner-Type Trap for Particulate Matter from a Diesel Engine," *Combust. Flame* 114, 585-590 (1998).

Diesel Engine
Ceramic
Regenerating
Soot Trap

20. PLUME/STACK CHEMISTRY/ATMOSPHERIC EMISSIONS

77850. Seinfeld, J.H., and S.N. Pandis, *"Atmospheric Chemistry and Physics: From Air Pollution to Climate Change,"* 1326 pp., John Wiley, New York NY (1998).

Atmospheric
Chemistry
Physics
Extensive
Textbook

77851. Fox, D.L., "Air Pollution," *Anal. Chem.* 69, 1R-13R (1997). | Air Pollution Gases/Aerosols 1995/1996 Literature Review

77852. Molina, M.J., L.T. Molina and C.E. Kolb, "Gas Phase and Heterogeneous Chemical Kinetics of the Troposphere and Stratosphere," *Ann. Rev. Phys. Chem.* 47, 327-367 (1996). | Troposphere Stratosphere Homo-, Heterogeneous Processes Review

77853. Rockmann, T., C.A.M. Brenninkmeijer, G. Saueressig, P. Bergamaschi, J.N. Crowley, H. Fischer and P.J. Crutzen, "Mass-Independent Oxygen Isotope Fractionation in Atmospheric CO as a Result of the Reaction CO+OH," *Science* 281, 544-546 (1998). | Atmospheric CO Isotopic Fractionations CO+OH Reaction Role

(78118) Atmospheric Chemistry, Lifetimes | $C_4F_9OC_2H_5$

(77957) Atmospheric Lifetimes, Ultraviolet-Visible Absorption Cross Sections | HOBr

77854. Pacyna, J.M., "Emission Inventories of Atmospheric Mercury from Anthropogenic Sources," in *Global and Regional Mercury Cycles: Sources, Fluxes and Mass Balances*, W. Baeyens, R. Ebinghaus and O. Vasiliev, eds., 30 Papers Presented at Novosibirsk, Russia, July 1995, 563 pp., NATO *Adv. Study Instit. Ser. Ser. 2: Environment* 21, 161-177 (1996). | Atmospheric Hg Anthropogenic Sources Review

(77875) Potential NO_x Formation Channel, Atmospheric Implications | $O_2(B)+N_2$

77855. Houghton, J., *"Global Warming: The Complete Briefing,"* 2nd Edition, 251 pp., Cambridge University Press, Cambridge UK (1997). | Climatic Impact Global Warming Briefing Handbook

77856. Kaufman, Y.J., and R.S. Fraser, "The Effect of Smoke Particles on Clouds and Climate Forcing," *Science* 277, 1636-1639 (1997). | Climatic Impact Biomass Burning Smoke Particle Effects

77857. Kaufmann, R.K., "Assessing the DICE Model: Uncertainty Associated with the Emission and Retention of Greenhouse Gases," *Climatic Change* 35, 435-448 (1997). | Climatic Impact Greenhouse Gases Model Assessment

77858. Kacholia, K., and R.A. Reck, "Comparison of Global Climate Change Simulations for Doubled CO_2 Induced Warming," *Climatic Change* 35, 53-69 (1997). | Climatic Impact CO_2 Modeling Efforts Uncertainties Review

77859. King, A.W., W.M. Post and S.D. Wullschleger, "The Potential Response of Terrestrial Carbon Storage to Changes in Climate and Atmospheric CO_2," *Climatic Change* 35, 199-227 (1997).

Climatic Impact
CO_2
Atmosphere/
Stored Carbon
Equilibrium
Changes
Modeling

21. COMBUSTION EMISSIONS/NO_X, SO_2 CHEMISTRY, CONTROL

(See also Section 19 for Engine Emissions)

77860. Van Vorst, W.D., and R.S. George, "Impact of the California Clean Air Act," *Int. J. Hydrogen Energy* 22, 31-38 (1997).

Combustion
Emissions
Clean Air Act
California
Trends

77861. Cofer III, W.R., K.P. Koutzenogii, A. Kokorin and A. Ezcurra, "Biomass Burning Emissions and the Atmosphere," in *Sediment Records of Biomass Burning and Global Change*, J.S. Clark, H. Cachier, J.G. Goldammer and B. Stocks, eds., 22 Papers Presented at a Workshop Held in Algarve, Portugal, October 1994, 489 pp., *NATO Adv. Sci. Instit. Ser. I. Global Environmental Change* 51, 189-206 (1997).

Biomass
Combustion
Atmospheric
Emissions
Particulates

77862. Novakov, T., H. Cachier, J.S. Clark, A. Gaudichet, S. Macko and P. Masclet, "Characterization of Particulate Products of Biomass Combustion," in *Sediment Records of Biomass Burning and Global Change*, J.S. Clark, H. Cachier, J.G. Goldammer and B. Stocks, eds., 22 Papers Presented at a Workshop Held in Algarve, Portugal, October 1994, 489 pp., *NATO Adv. Sci. Instit. Ser. I. Global Environmental Change* 51, 117-143 (1997).

Biomass
Combustion
Particulate
Analysis
Sizes

77863. *"Waste Combustion in Boilers and Industrial Furnaces," Proceedings of an International Specialty Conference*, Held in Clearwater FL, March 1993, 27 Papers, 313 pp., Air and Waste Management Association, Pittsburgh PA (1993).

Incineration
Wastes
Conference
Proceedings

77864. *"Waste Combustion in Boilers and Industrial Furnaces," Proceedings of an International Specialty Conference*, Held in Kansas City MO, April 1994, 27 Papers, 318 pp., Air and Waste Management Association, Pittsburgh PA (1994).

Incineration
Wastes
Emissions Control
Conference
Proceedings

77865. Akhmetzyanov, A.M., V.F. Kharitonov, E.Z. Sirayev, K.S. Gumerov and A.F. Ivakh, "Commercial Hazardous Liquid Waste Disposers Using Thermojet Afterburners," *Russ. Aeronaut.* 38(1), 95-100 (1995).

Incineration
Thermojet
Afterburner
Liquid Wastes
Effectiveness

77866. Penetrante, B.M., M.C. Hsiao, J.N. Bardsley, B.T. Merritt, G.E. Vogtlin, A. Kuthi, C.P. Burkhart and J.R. Bayless, "Decomposition of Methylene Chloride by Electron Beam and Pulsed Corona Processing," *Phys. Lett. A* 235, 76-82 (1997).

Incineration
CH_2Cl_2/Air,N_2
e-Beam/
Discharge Methods
Products

77867. Ravindran, V., M. Pirbazari, S.W. Benson, B.N. Badriyha and D.H. Evans, "Thermal Destruction of Chlorinated Hydrocarbons by Reductive Pyrolysis," *Combust. Sci. Technol.* 122, 183-213 (1997).

Incineration
Pyrolytic
CH_3Cl,PCBs
Flow Reactor
Efficiencies

77868. Kashireninov, O.E., and A. Fontijn, "Modeling of Chromium Combustion in Incineration: Thermochemistry of Cr-C-H-Cl Combustion in Air and Selection of Key Reactions," *Combust. Flame* 113, 498-506 (1998).

Incineration
Cr
Gaseous Speciation
Equilibrium
Calculations

77869. Antsiferov, V.N., M.Yu. Kalashnikova, A.M. Makarov, S.E. Porozova and I.V. Filimonova, "Block Catalysts Based on Highly Porous Cellular Materials for Afterburning of Hydrocarbons and Carbon Monoxide," *Russ. J. Appl. Chem.* 70, 104-107 (1997).

Emissions Control
CO,Organics
Porous
Cellular Catalysts
Efficiencies

(77662) Emissions, Sintered Metal Burner, CH_4 Catalytic Combustion, Model

CO,NO

77870. Dagaut, P., and M. Cathonnet, "A Comparative Study of the Kinetics of Benzene Formation from Unsaturated C_2 to C_4 Hydrocarbons," *Combust. Flame* 113, 620-623 (1998).

C_6H_6 Formation
C_2H_2 ,C_3H_4/O_2
C_3H_6 ,C_4H_6/O_2
Jet Stirred
Reactor

77871. Lukachev, S.V., S.G. Matveev and A.F. Uryvskii, "On Modeling Benz(*a*)Pyrene Formation Process Based on Global Reactions," *Russ. Aeronaut.* 39(1), 60-62 (1996).

PAH
Formation
Rich Combustion
Kinetic Modeling

77872. Vincitore, A.M., and S.M. Senkan, "Polycyclic Aromatic Hydrocarbon Formation in Opposed Flow Diffusion Flames of Ethane," *Combust. Flame* 114, 259-266 (1998).

PAH,Aromatics
Formation
C_2H_6/O_2/Ar
Opposed Flow
Diffusion Flames
Probe Sampling
Species Profiles

(78092) Formation, *n*-C_4H_{10}/O_2/Ar, Species Profiles, Kinetic Modeling, Data Comparisons

PAH,Aromatics

77873. Vecera, Z., and P.K. Dasgupta, "Indoor Nitrous Acid Levels: Production of Nitrous Acid from Open Flame Sources," *Int. J. Environ. Anal. Chem.* 56, 311-316 (1994).

HONO
Formation
Indoor
Flame Sources
Levels

77874.	Treanor, C.E., I.V. Adamovich, M.J. Williams and J.W. Rich, "Kinetics of Nitric Oxide Formation Behind Shock Waves," Paper Published Originally as AIAA Paper 95-2061 at the *29th AIAA Thermophysics Conference*, Held in San Diego CA, June 1995, *J. Thermophys. Heat Transfer* 10, 193-199 (1996).	NO Formation N_2/O_2 Shock Discharge Zeldovich Mechanism Vibrational Nonequilibrium Effects
77875.	Zipf, E.C., and S.S. Prasad, "Evidence for New Sources of NO_x in the Lower Atmosphere," *Science* 279, 211-213 (1998).	NO_x Formation $O_2(B)+N_2$ Potential Channel Atmospheric Implications
77876.	Chen, R.-H., J.E. Navedo and L. Chew, "Effects of Fuel Lewis Number on and Damkohler Number Scaling of Nitric Oxide Emission Level of Burke-Schumann Type Flames," *Combust. Sci. Technol.* 127, 293-318 (1997).	NO Formation Burke-Schumann Diffusion Flames Damkohler Number Correlations
77877.	Hsieh, T.-C.A., W.J.A. Dahm and J.F. Driscoll, "Scaling Laws for NO_x Emission Performance of Burners and Furnaces from 30 kW to 12 MW," *Combust. Flame* 114, 54-80 (1998).	NO_x Formation Swirl Stabilized Burners/Furnaces General Scaling Laws
77878.	Newburry, D.M., and A.M. Mellor, "Semiempirical Correlations of NO_x Emissions from Utility Combustion Turbines with Inert Injection," *J. Propulsion Power* 12, 527-533 (1996).	NO_x Formation Turbines Inert Injection Semiempirical Correlations Model
77879.	Broadwell, J.E., and A.E. Lutz, "A Turbulent Jet Chemical Reaction Model: NO_x Production in Jet Flames," *Combust. Flame* 114, 319-335 (1998).	NO_x Formation Turbulent CH_4,CO/H_2 H_2 Jet Flames Model
77880.	Ju, Y., and T. Niioka, "Computation of NO_x Emission of a Methane/Air Diffusion Flame in a Two-Dimensional Laminar Jet with Detailed Chemistry," *Combust. Theory Modeling* 1, 243-258 (1997).	NO Formation CH_4/Air 2-D Jet Kinetic Modeling Prompt/Thermal Contributions
77881.	Hayhurst, A.N., and E.M. Hutchinson, "Evidence for a New Way of Producing NO via NNH in Fuel-Rich Flames at Atmospheric Pressure," *Combust. Flame* 114, 274-279 (1998).	NO_x Formation Fuel Rich CH_4,$H_2/O_2/N_2$ Flame Profiles N_2H Role

77882.	Dupont, V., and A. Williams, "NO_x Mechanisms in Rich Methane/Air Flames," *Combust. Flame* 114, 103-118 (1998).	NO_x Formation Co-flow Rich CH_4/Air Double Flame T,CARS OH,LIF Mechanisms
(77771)	Formation, Turbulent C_2H_4, C_3H_8, H_2 Co-flow Air Diffusion Flames	NO,NO_2,Soot
(77668)	Turbulent Swirling Pulverized Coal Combustor, Numerical Model	NO Formation
(77742)	H_2/Air, Partially Stirred Reactor, Unmixedness Combustion Effects, Modeling	NO Formation
77883.	Bowman, C.T., "Mechanisms and Modeling of Gas Phase Aftertreatment Methods for NO Removal from Combustion Products," pp. 29-68 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	NO_x Control Thermal $DeNO_x$ $RAPRENO_x$ Mechanisms Kinetic Modeling Sensitivity Analyses Review
(78224)	HN_2 /H+N_2 Reaction Dynamics, Exothermicity, Barrier Height, Calculations	$DeNO_x$ Kinetics
77884.	Faravelli, T., A. Antichi, C. Callierotti, E. Ranzi and D. Benedetto, "A Kinetic Study of an Advanced Reburning Process," *Combust. Theory Modeling* 1, 377-393 (1997).	NO_x Control NH_3,HNCO Relative Effectiveness Comparisons Kinetic Modeling
77885.	Hasegawa, T., and M. Sato, "Study of Ammonia Removal from Coal-Gasified Fuel," *Combust. Flame* 114, 246-258 (1998).	NO_x Control Coal Syngas Optimal NO/NH_3 Ratios CH_4,CO,H_2,O_2 Effects
77886.	Rota, R., F. Bonini, A. Servida, M. Morbidelli and S. Carra, "Modeling of the Reburning Process," *Combust. Sci. Technol.* 123, 83-105 (1997).	NO_x Control Reburn Method Fluid Dynamics/ Kinetic Model Data Comparisons
77887.	Dahiya, R.P., S.K. Mishra and A. Veefkind, "Plasma Chemical Investigations for NO_x and SO_2 Removal from Flue Gases," *IEEE Trans. Plasma Sci.* 21, 346-348 (1993).	NO,NO_2,SO_2 Control Discharge Method Major Kinetic Channels

77888.	Hensel, K., and M. Morvova, "The Conversion of NO_x in a Corona Discharge with an Electrode Material Variation," *Contrib. Plasma Phys.* 36, 51-61 (1996).	NO_x Control Corona Discharge Method Electrode Material Effects
77889.	Jaworek, A., A. Krupa and T. Czech, "Decomposition of NO_2 in Oxygen Free NO_2:N_2 Gas Mixture by Back Corona Generated Plasma," *Contrib. Plasma Phys.* 36, 619-629 (1996).	NO_2/N_2 Dissociation Back Corona Discharge Method

22. SOOT, DIAMOND, PARTICLE FORMATION/CONTROL

(See also Section 19 for Engine Soot Formation)

77890.	Naegeli, D.W., "Effects of Diluents and Temperature on Soot Inception in Premixed Flames," pp. 253-263 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Soot Formation Flame Temperature Effects 7 Hydrocarbon Fuels
77891.	Takahashi, F., "Sooting Correlations for Premixed Combustion," pp. 161-187 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Soot Formation Threshold Data Analysis Fuel/O_2 Ratio Correlation
77892.	Hall, R.J., M.D. Smooke and M.B. Colket, "Predictions of Soot Dynamics in Opposed Jet Diffusion Flames," pp. 189-230 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Soot Formation Opposed Jet CH_4 Diffusion Gas/Particle Flame Modeling
77893.	Dobbins, R.A., "The Early Soot Particle Formation in Hydrocarbon Flames," pp. 107-133 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Soot Formation Precursor Small Particle Sampling Characterization
77894.	Sadakata, M., M. Motegi, Y. Mashio, T. Ishida, A. Harano and H.J. Kim, "Growth of Primary Soot Particles in an Atmospheric Premixed Methane Oxygen Flame," *Chem. Eng. Res. Design. Trans. Inst. Chem. Eng.* 73, 142-146 (1995).	Soot Growth CH_4/O_2 Post Flame Sampling PAHS $C_{14}H_{10}$, C_2H_2 Injection Effects

77895.	Hwang, J.Y., W. Lee, H.G. Kang and S.H. Chung, "Synergistic Effect of Ethylene/Propane Mixture on Soot Formation in Laminar Diffusion Flames," *Combust. Flame* 114, 370-380 (1998).	Soot,PAH Formation C_2H_4/C_3H_8 C_2H_4/C_2H_6 Synergistic Effects
(77679)	Spray Combustion, Electrostatic Dispersion, Size Effects	Soot Formation
77896.	Dunai, O.V., O.V. Strogonov, V.Yu. Naumov and V.A. Shchukin, "Experimental Study of Soot Particle Ejection at Burning of Nonuniform Homogeneous Kerosene/Air Mixture in Turbulent Flow," *Russ. Aeronaut.* 37(4), 37-41 (1994).	Soot Formation Turbulent Combustor Kerosene/Air Nonuniform Mixture Effects
77897.	Avedisian, C.T., "Soot Formation in Spherically Symmetric Droplet Combustion," pp. 135-160 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).	Soot Formation Droplet Combustion Microgravity $C_6H_5CH_3/CH_3OH$ Soot Shells
77898.	Jacob, K.T., N. Gundiah and A.G. Menon, "A Thermodynamic Criterion for Selection of Gas Compositions for Diamond Deposition," *High Temp. Mater. Process.* 15, 223-235 (1996).	Diamond Formation CVD C/H/O Systems Thermodynamic Optimizations
77899.	Rakov, E.G., "Calculation of Diamond Deposition Fields in the Phase Diagrams of the C-H-O, C-H-O-F and C-S-F Systems," *Dokl. Phys. Chem.* 349, 178-181 (1996).	Diamond Formation C/H/O;C/S/F C/H/O/F Thermochemical Calculations T,Concentration Parameters
77900.	Menningen, K.L., M.A. Childs, H. Toyoda, Y. Ueda, L.W. Anderson and J.E. Lawler, "CH_3 and CH Densities in a Diamond Growth DC Discharge," *Contrib. Plasma Phys.* 35, 359-373 (1995).	Diamond Formation CH_4/H_2 Plasma Discharge CH,CH_3 Density Measurements
(77905)	Atmospheric Nucleation, Review	Particle Formation
77901.	Kasper, M., K. Siegmann and K. Sattler, "Evaluation of an in Situ Sampling Probe for Its Accuracy in Determining Particle Size Distributions from Flames," *J. Aerosol Sci.* 28, 1569-1578 (1997).	Particle Formation CH_4/Air Pd,Pt Seeding Soot Sampling Probe Size Distributions Method

77902. Lindackers, D., M.G.D. Strecker, P. Roth, C. Janzen and S.E. Pratsinis, "Formation and Growth of SiO_2 Particles in Low Pressure $H_2/O_2/Ar$ Flames Doped with SiH_4," *Combust. Sci. Technol.* 123, 287-315 (1997).

SiO_2
Particle Formation
$H_2/O_2/Ar/SiH_4$
Low Pressure Flames
Sizes/
Distribution

77903. Burov, Yu.M., Yu.M. Grigor'ev and S.G. Kuz'minskaya, "Thermodynamic Study of Synthesis of Titanium Boride by the Method of Condensation Combustion of Gases," *Combust. Expl. Shock Waves, Russia* 33, 548-552 (1997).

TiB, TiB_2
Formation
$Na/TiCl_4$
$Na/BCl_3/TiCl_4$
Equilibrium
Calculations
Products

23. PARTICLE CHARACTERIZATION

(See also Section 5 for Spray Characterization)

(77862) Biomass Combustion Particulates, Analysis

Sizes

(77901) Particle Formation, CH_4/Air, Pd, Pt Seeding, Soot Formation, Sampling Probe, Internal Comparative Technique

Size Distributions

77904. Fan, J., H. Zhao and K. Cen, "Particle Concentration and Size Measurements in Two-Phase Turbulent Coaxial Jets" *Chem. Eng. Commun.* 156, 115-129 (1996).

Particle
Sizes,Densities
2-Phase
Turbulent
Coaxial Jet
Tomographic
LDM Method

24. NUCLEATION/COAGULATION/CLUSTERS

(See also Section 26 for Spectroscopy of Cluster Molecules)

77905. Laaksonen, A., V. Talanquer and D.W. Oxtoby, "Nucleation: Measurements, Theory and Atmospheric Applications," *Ann. Rev. Phys. Chem.* 46, 489-524 (1995).

Nucleation
Atmospheric
Particle Formation
Review

77906. Uchtmann, H., R. Dettmer, S.D. Baranovskii and F. Hensel, "Photoinduced Nucleation in Supersaturated Mercury Vapor," *J. Chem. Phys.* 108, 9775-9782 (1998).

Nucleation
Hg Vapor
Photoinduced
Rates

77907. Kazakov, A., and M. Frenklach, "Dynamic Modeling of Soot Particle Coagulation and Aggregation: Implementation with the Method of Moments and Application to High Pressure Laminar Premixed Flames," *Combust. Flame* 114, 484-501 (1998).

Soot
Coagulation
Aggregation
C_2H_4/Air
Improved Model

77908.	Jouvet, C., and D. Solgadi, "Photochemistry of van der Waals Complexes and Small Clusters," pp. 100-146 in *Chemical Reactions in Clusters*, E.R. Bernstein, ed., 7 Contributions, 261 pp., Oxford University Press, New York (1996).	Clusters Photochemistry Review
(78296)	Dimers, Trimers, Structural Calculations, Geometries, Frequencies	$\Delta H_f(Al(CH_3)_2H)$ $\Delta H_f(Al(CH_3)_3)$
(78265)	MPI, fs Pulses, Product Ion Energies	$Ar_n,(CH_3COCH_3)_n$
(78308)	Structural Calculations, Geometries, Frequencies, Excitation Energies	$CH_2O.HF$
77909.	Wittig, C., and A.H. Zewail, "Dynamics of Ground State Bimolecular Reactions," pp. 64-99 in *Chemical Reactions in Clusters*, E.R. Bernstein, ed., 7 Contributions, 261 pp., Oxford University Press, New York (1996).	Clusters $CO_2.HX+h\nu$ $H+CO_2$ $HBr.I_2+h\nu$ $Br+I_2$ Dynamical Effects Review
77910.	Dunne, L.J., P.F. Nolan, M. Terrones, J. Munn, A. Jones, P. Kathirgamanathan and J. Fernandez, "Formation of Twisted AB-Graphitic and Fullerene-Related Tubular Structures During Soot Deposition from the Flaming Combustion of Polymers," *Combust. Flame* 114, 591-593 (1998).	Fullerenes AB-Graphitic Formation Polymer Combustion
77911.	Deng, R., and O. Echt, "Efficiency of Thermionic Emission from C_{60}," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2533-2539 (1998).	C_{60} Thermionic Emission 355 nm Induced Delayed Electron Efficiency
(78326)	Bond Energies, Structural Calculations	C_{60},C_{70} C_{76},C_{78}
(78120)	Rate Constants, Temperature Dependences, Shock Tube	$C_{60}+H,OH$
(77800)	C_2 Elimination, Transition State Dynamics, Measurements	C_{60}^+
(78149)	UV/Visible Fragmentation Patterns, 24 PAHS	$C_{60}^++h\nu$ $PAH^++h\nu$
(78171)	CaCl(X,v) Product State Distributions, P.E. Surfaces, Dynamics, Measurements	$Ca.HCl+h\nu$
(78152)	Product MPI Fragmentation Patterns	$Cr(CO)_6+h\nu$ $Cr(CO)_6.(CH_3OH)_n+h\nu$
(77801)	Reactive Cross Sections, n=1-18, Product Ions, $D(Cr_n^+O)$	$Cr_n^++CO_2$
(77802)	Reactive Cross Sections, n=2-18, Product Ions, $D(Cr_mO_2^+)$	$Cr_n^++O_2$
(78333)	Bonding Energies, Geometries, Structural Calculations	F_4^+

(78153)	Photodissociation Dynamics, Channels, Products	$HCl.Ar + h\nu$
(78392)	Calculations	$\Delta H_f(H_2O)_2$
(78025)	Predissociation Rate Constants, Rg=Ne,Ar,Kr, $I_2(B,v)$ Products, Calculations	$I_2(B).Rg$
(78179)	RH=CH_4,C_2H_6,C_3H_8, OH(v=0,1,J) Product Distributions, Comparisons, Cluster Effects	$N_2O.RH + h\nu$ $O(^1D) + RH$
(78157)	Trajectory Calculations, Cluster Effects	$NaI(H_2O) + h\nu$
77912.	Berces, A., P.A. Hackett, L. Lian, S.A. Mitchell and D.M. Rayner, "Reactivity of Niobium Clusters with Nitrogen and Deuterium," *J. Chem. Phys.* 108, 5476-5490 (1998).	$Nb_n + D_2, N_2$ Rate Constants n=2-20
(77808)	Rate Constants, n=2-7, Absorption/Fragmentation	$Nb_n^- + CO, N_2$
(77809)	Relative Rate Constants, n=3-28	$Nb_n^- + C_6H_6$ $Rh_n^- + C_6H_6$
(78178)	OH(J) Product Energy Distributions, Cluster Effects	O+HCl.Ar $O(^1D)$+HCl.Ar
(78243)	Reaction Dynamics, P.E. Surfaces, Low-lying States, Calculations	$Pd_2 + H_2$ $Pd_3 + H_2$
(78244)	Reaction Dynamics, Channels, Reactivities, Energetics, Calculations	$Pt,Pt_2 + CH_4, H_2$ $Pd,Pd_2 + CH_4, H_2$
(77813)	n=2-17, Channels, Energy Dependences, $D(V_n^+\text{-}O)$, n=2-15	$V_n^+ + O_2$

25. FLAME/CHEMILUMINESCENT SPECTROSCOPY

(77737)	Diffusion Flames, Model Comparisons	Radiative Heat Transfer
(77766)	Turbulent C_2H_2/Air, Linear Eddy Model	Soot/Radiation Interactions
(78000)	Chemiluminescence, $Ba(^3D_J) + CF_2Br_2$, CF_3Br, Branching Ratios	BaBr(B,A-X)
(78001)	Chemiluminescence, $Ba(^3D_J) + CH_3I$, Branching Ratios	BaI(B,A-X)
77913.	Kampf, R.P., and J.M. Parson, "Chemiluminescent Pathways in Reactions of Phosphorus, Antimony and Bismuth with Ozone to Form Dioxides and Monoxides," *J. Chem. Phys.* 108, 7595-7606 (1998).	Chemiluminescence PO_2^*,SbO*,SbO_2^* BiO*,BiO_2^* $P,Bi + O_3$ $Sb,Sb_2 + O_3$ Molecular Beams

26. SPECTRAL CHARACTERIZATIONS/ANALYSES

(See also Section 43 for Energy Levels and Theoretically Calculated Spectral Constants, and Section 44 for Vibrational Frequencies and Constants)

77914.	van Duijnen, P.T., and M. Swart, "Molecular and Atomic Polarizabilities: Thole's Model Revisited," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2399-2407 (1998).	Polarizabilities Molecular Estimation Model
77915.	Wiese, W.L., "Atomic Spectroscopic Databases on the World Wide Web," *Spectrochim. Acta B. At. Spectrosc.* 52, 279-280 (1997).	Atomic Spectroscopy Databases Review
(78078)	Atoms, Molecules, Tabulations of Studies, Review	Optogalvanic Spectroscopy
77916.	Schlag, E.W., *"ZEKE Spectroscopy,"* 277 pp., Cambridge University Press, Cambridge UK (1998).	ZEKE Spectroscopy Primer Handbook
77917.	Wang, K., and V. McKoy, "High Resolution Photoelectron Spectroscopy of Molecules," *Ann. Rev. Phys. Chem.* 46, 275-304 (1995).	Photoelectron Rotationally Resolved Spectra CH_2O,CH_3,CO HBr,H_2O NO,N_2,OH Photoionization Review
77918.	Ren, J., M.-H. Whangbo, D. Dai and L. Li, "Description of Ligand Field Splitting in Terms of Density Functional Theory: Split Levels of the Lowest-lying Subterms of the $4f^{n-1}6s^2$ (n=3-14) Configurations in Lanthanide Monofluorides LnF (Ln=Pr-Yb)," *J. Chem. Phys.* 108, 8479-8484 (1998).	MF Lanthanides M=Pr-Yb Low-lying Electronic States Sub-level Energies Calculation Method
77919.	Steimle, T., M. Tanimoto, K. Namiki and S. Saito, "The Millimeter Wave Spectrum of Silver Monoxide, AgO," *J. Chem. Phys.* 108, 7616-7622 (1998).	AgO Rotational Spectra Constants
77920.	Ruschel, G.K., and D.W. Ball, "Matrix Isolation and Density Functional Studies of Novel Metal Complexes: Al+NO in Solid Argon," *High Temp. Mater. Sci.* 37, 63-70 (1997).	AlNO FTIR Spectrum Matrix Isolation Study

77921.	Herring, C.M., J.G. Eden and M.L. Ginter, "The ($5f\pi^3\Pi_g \leftarrow a^3\Sigma_u^+$) and ($5f\sigma^3\Sigma_g^+ \leftarrow a^3\Sigma_u^+$) Systems of Ar_2," *J. Chem. Phys.* 108, 5426-5431 (1998).	Ar_2(5f-a) Laser Excitation Spectra Assignments Constants
77922.	Yang, S.-F., X.-g. Wang and Q.-S. Zhu, "High Resolution Vibration-Rotation Spectrum of Arsine v=2 Stretching Overtone," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 157-163 (1997).	$AsH_3(2\nu_1,\nu_1+\nu_3)$ FTIR Overtone Spectrum Constants
77923.	Nomoto, M., T. Okabayashi, T. Klaus and M. Tanimoto, "Microwave Spectroscopic Study of the BBr Molecule," *J. Mol. Struct.* 413/414, 471-476 (1997).	BBr Rotational Spectrum Constants B/O Breakdown
77924.	Andrews, L., D.V. Lanzisera, P. Hassanzadeh and Y. Hannachi, "Reactions of Laser Ablated Boron Atoms with Ethylene and Ethane: Infrared Spectra and DFT Calculations for Several Novel BC_2H_x (x=1,2,3,4,5) Molecules," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3259-3267 (1998).	BC_2H_n,n=1-5 FTIR Product Analysis Laser Ablation $B+C_2H_4,C_2H_6$ Matrix Study
77925.	Agreiter, J., M. Lorenz, A.M. Smith and V.E. Bondybey, "Neon Matrix Spectra and Isotopically Dependent Fluorescence Quantum Yields of BO_2," *Chem. Phys.* 224, 301-313 (1997).	BO_2(A-X) LIF Quantum Yields Isotopomers Structure Matrix Study
77926.	Habara, H., S. Yamamoto, C. Ochsenfeld, M. Head-Gordon, R.I. Kaiser and Y.T. Lee, "Fourier Transform Millimeter-Wave Spectroscopy of the HCS Radical in the $^2A'$ Ground Electronic State," *J. Chem. Phys.* 108, 8859-8863 (1998).	HCS(X) FT Millimeter Wave Spectrum Structure Constants
(78376)	Photoionization Spectral Measurements, IP(CH_2), $\Delta H_f(CH_2$(a,X)) and $D_0(CH_3)$	$CH_2(X^3B_1)$
77927.	Osmann, G., P.R. Bunker, P. Jensen and W.P. Kraemer, "A Theoretical Calculation of the Absorption Spectrum of CH_2^+," *Chem. Phys.* 225, 33-54 (1997).	CH_2^+(A-X) Absorption Spectrum Lines,Intensities D-Isotopes Calculations
77928.	Cavagnat, D., and L. Lespade, "Vibrational Overtone Spectroscopy and Internal Dynamics in Gaseous Nitromethane NO_2CH_2D," *J. Chem. Phys.* 108, 9275-9284 (1998).	$CH_2DNO_2(1\text{-}6\nu_{CH})$ FTIR Intracavity Laser Optoacoustic Spectra Frequencies

77929.	Courtecuisse, S., F. Cansell, D. Fabre and J.P. Petitet, "Comparative Raman Spectroscopy of Nitromethane-*h*$_3$, Nitromethane-*d*$_3$, and Nitroethane up to 20 GPa," *J. Chem. Phys.* 108, 7350-7355 (1998).	CH_3NO_2 ,CD_3NO_2 $C_2H_5NO_2$ Raman Spectra High Pressures Detonation Regime
77930.	Bagaev, S.N., A.S. Dychkov, Yu.A. Matyugin and N.V. Fateev, "Laser Spectroscopy of the $2\nu_3$ Band of Methane," *Opt. Spectrosc., Russia* 83, 79-83 (1997).	CH_4 ,$2\nu_3$ Spectrum Constants Absorption Coefficient
77931.	Sykora, T., and C.R. Vidal, "Interaction of a Magnetic Field with the (a′ $^3\Sigma^+$/A$^1\Pi$) Complex in CO," *J. Chem. Phys.* 108, 6320-6330 (1998).	CO(a′-X) Absorption Field Effects a′/A State Mixing a′(v=14,N) Lifetimes
(78382)	Photoelectron Spectra, IP, Spin-Orbit Splitting, Vibronic Levels, Experiment/Theory	COS^+
77932.	Dyke, J.M., S.D. Gamblin, D. Haggerston, A. Morris, S. Stranges, J.B. West, T.G. Wright and A.E. Wright, "A Study of the CS Molecule with Photoelectron Spectroscopy Using Synchrotron Radiation," *J. Chem. Phys.* 108, 6258-6265 (1998).	CS Photoelectron Spectra CS^+(X)Constants
77933.	Leininger, M.L., C.D. Sherrill, W.D. Allen and H.F. Schaefer III, "Benchmark Configuration Interaction Spectroscopic Constants for $C_2(X^1\Sigma_g^+)$ and $CN^+(X^1\Sigma^+)$," *J. Chem. Phys.* 108, 6717-6721 (1998).	C_2(X),CN^+(X) Spectral Constant Calculations
77934.	Guirgis, G.A., Y. Jin, P. Klaeboe and J.R. Durig, "Infrared and Raman Spectra, Conformational Stability, Barriers to Internal Rotation, ab Initio Calculations and Vibrational Assignments for Dichlorofluoroacetyl Fluoride," *Chem. Phys.* 223, 131-148 (1997).	CCl_2FCFO IR,Raman Spectra Structural Calculations Geometries Frequency Assignments
(78385)	Threshold Photoelectron Spectra, IP(*c*-C_4F_8), $\Delta H_f(C_3F_5^+)$, Measurements	C_2F_4 ,C_3F_6 2-C_4F_8 ,*c*-C_4F_8
(78375)	Threshold Photoelectron Spectra, IP(CF_3), $\Delta H_f(C_3F_7^+)$	C_2F_6 ,C_3F_8 ,C_4F_{10}
77935.	Maier, J.P., "Electronic Spectroscopy of Carbon Chains, "*J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3462-3469 (1998).	C_n ,C_n^- C_nH,HC_nH^+ Absorption Spectra Matrix Study

77936. Taylor, T.R., C. Xu and D.M. Neumark, "Photoelectron Spectra of the $C_{2n}H^-$ (n=1-4) and $C_{2n}D^-$ (n=1-3) Anions," *J. Chem. Phys.* 108, 10018-10026 (1998).

$C_{2n}H^-$,n=1-4
$C_{2n}D^-$,n=1-3
Photoelectron Spectra
Assignments

77937. O'Brien, J.P., M.P. Jacobson, J.J. Sokol, S.L. Coy and R.W. Field, "Numerical Pattern Recognition Analysis of Acetylene Dispersed Fluorescence Spectra," *J. Chem. Phys.* 108, 7100-7113 (1998).

C_2H_2(A-X)
LIF
Vibrational Level Assignments

77938. Moazzen-Ahmadi, N., and R.T. Boere, "Infrared Diode Laser Spectroscopy of the CCO Radical: The ($2\nu_1$-ν_1) and ($\nu_1+\nu_3$-ν_3) Difference Bands," *J. Chem. Phys.* 108, 6588-6593 (1998).

C_2O
IR Spectra
ν_1,($2\nu_1$-ν_1)
Constants

77939. Fulara, J., M. Grutter, M. Wyss and J.P. Maier, "($A^2\Sigma^+ \leftarrow X^2\Pi$) Electronic Absorption Spectrum of CCO^- in a Neon Matrix," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3459-3461 (1998).

C_2O^-(A-X)
Absorption Spectrum
Frequencies
Matrix Study

77940. Cermak, I., M. Forderer, I. Cermakova, S. Kalhofer, H. Stopka-Ebeler, G. Monninger and W. Kratschmer, "Laser Induced Emission Spectroscopy of Matrix-Isolated Carbon Molecules: Experimental Setup and New Results on C_3," *J. Chem. Phys.* 108, 10129-10142 (1998).

C_3(a,A-X)
LIF
Phosphorescence
A-State Lifetime
Matrix Study

77941. Williams, S., E. Zingher and J.C. Weisshaar, "(B←X) Vibronic Spectra and B-State Fluorescence Lifetimes of Methylvinoxy Isomers," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2297-2301 (1998).

CH_2COCH_3(B-X)
LIF Spectra
B-State Lifetimes
Isomers

(78116) Absorption Cross Section Measurements

c-$C_3H_5O_3$,(*c*-$C_3H_5O_3$)O_2
UV Spectra
(*c*-$C_3H_5O_3$)O_2NO_2
IR Spectrum

77942. Zheng, X., and D.L. Phillips, "Effect of Geometrical Conformation on the Short-Time Photodissociation Dynamics of 1-Iodopropane in the A-Band Absorption," *J. Chem. Phys.* 108, 5772-5783 (1998).

1-C_3H_7I
RRS
Raman Cross Sections
A-Band Absorption Measurements

77943. Khlifi, M., P. Paillous, P. Bruston, J.C. Guillemin, Y. Benilan, A. Daoudi and F. Raulin, "Gas Infrared Spectra, Assignments and Absolute Infrared Band Intensities of C_4N_2 in the 250-3500 cm^{-1} Region: Implications for Titan's Stratosphere," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 707-712 (1997).

C_4N_2
FTIR Spectrum
Assignments
Band Intensities

77944.	Troxler, T., "(S_1-S_0) Electronic Spectroscopy and ab Initio Calculations of *cis*-2-Methoxynaphthalene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4775-4787 (1998).	*cis*-2-$C_{10}H_7OCH_3$ LIF Spectrum Geometry Frequencies Assignments
77945.	Kautz, I., T. Koch, K. Malsch and G. Hohlneicher, "Ground State Vibrations of Biphenylene: Experiment and Theory," *J. Mol. Struct.* 417, 223-236 (1997).	$C_6H_4C_6H_4$ FTIR Spectra Frequencies Matrix Study
77946.	Negri, F., and G. Orlandi, "Vibronic Structure in the Multiple State Fluorescence Spectrum of C_{70} : A Theoretical Investigation," *J. Chem. Phys.* 108, 9675-9684 (1998).	C_{70} LIF Spectrum Theoretical Analysis Assignments
77947.	Sassara, A., G. Zerza and M. Chergui, "Assignment of the Lowest Excited States of C_{70} and Evidence for Fluorescence from the S_2 State," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3072-3077 (1998).	C_{70} LIF Spectra Phosphorescence Assignments Matrix Study
77948.	France, M.R., S.H. Pullins and M.A. Duncan, "Spectroscopy of the Ca^+-Acetylene π Complex," *J. Chem. Phys.* 108, 7049-7051 (1998).	$Ca^+.C_2H_2$ Photodissociation Spectrum r_0'',ω_0'',D_0''
77949.	Morbi, Z., C. Zhao, J.W. Hepburn and P.F. Bernath, "High Resolution Visible Laser Spectroscopy of the (B^2B_1-X^2A_1) Transition of $CaNH_2$," *J. Chem. Phys.* 108, 8891-8898 (1998).	$CaNH_2$(B-X) LIF Spectrum Supersonic Beam Assignments
77950.	Andrews, L., A. Citra, G.V. Chertihin, W.D. Bare and M. Neurock, "Reactions of Laser Ablated Co and Ni Atoms with Nitrogen Atoms and Molecules: Infrared Spectra and DFT Calculations of Metal Nitride Molecular Species and Complexes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2561-2571 (1998).	CoN,NiN $(CoN)_2$,$(NiN)_2$ FTIR Spectra Frequencies Co,Ni/N_2 Laser Ablation Matrix Study
(78389)	Photoionization Spectra, D(Cr_2,Mo_2^+), IP(Cr_2,Mo_2)	Cr_2,Mo_2
77951.	Grantier, D.R., and J.L. Gole, "Chemically Induced Resonance Raman Scattering in Cesium Dimer," *Chem. Phys.* 223, 273-278 (1997).	Cs_2(A-X) RRS Spectrum Cs(^2P_J) Emission Pumping
77952.	Stangassinger, A., A.M. Knight and M.A. Duncan, "Photoionization Spectroscopy of Ga-Rare Gas Complexes," *J. Chem. Phys.* 108, 5733-5741 (1998).	GaRg(F,G,H,I) R2PI Spectra Rg=Ar,Kr,Xe Constants D_0',D_0''

77953. Zumbusch, A., and H. Schnockel, "Raman and Infrared Spectroscopy of $(GeO)_n$, with n=1-4, Isolated in Solid Argon," *J. Chem. Phys.* 108, 8092-8100 (1998).

$(GeO)_n$, n=1-4
IR, Raman Spectra
Geometries
Frequencies
Matrix Study

77954. Jung, M., B.P. Winnewisser and M. Winnewisser, "High Resolution FTIR Spectra of the ν_1, ν_2 and ν_3 Bands of $H^{12}CP$ and of the ν_1 and ν_2 Bands of $H^{13}CP$," *J. Mol. Struct.* 413/414, 31-48 (1997).

HCP, ν_1, ν_2, ν_3
FTIR Spectra
Assignments
Constants

77955. Chunhui, L., H. Gongyi, C. Benming, W. Dianxun and J.B. Peel, "He(I) Photoelectron Spectroscopic Study on the Electron Structure of Perchloric Acid, $HOClO_3$, and Fluorine Perchlorate, $FOClO_3$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3877-3879 (1998).

$HClO_4$
$FClO_4$
Photoelectron Spectral Assignments

77956. Donaldson, D.J., J.J. Orlando, S. Amann, G.S. Tyndall, R.J. Proos, B.R. Henry and V. Vaida, "Absolute Intensities of Nitric Acid Overtones," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5171-5174 (1998).

$HNO_3(3,4\nu_{OH})$
Overtone Transitions
Oscillator Strengths
Measurements

77957. Ingham, T., D. Bauer, J. Landgraf and J.N. Crowley, "Ultraviolet-Visible Absorption Cross Sections of Gaseous HOBr," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3293-3298 (1998).

HOBr
UV-Visible Absorption
Cross Sections
Atmospheric Lifetimes

77958. Bauer, D., T. Ingham, S.A. Carl, G.K. Moortgat and J.N. Crowley, "Ultraviolet-Visible Absorption Cross Sections of Gaseous HOI and Its Photolysis at 355 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2857-2864 (1998).

HOI
UV-Visible Absorption
Cross Sections
OH Product
Quantum Yields

77959. Roncin, J.-Y., and F. Launay, "Atlas of the Vacuum Ultraviolet Emission Spectrum of Molecular Hydrogen," *J. Phys. Chem. Ref. Data Monograph* No. 4, 417 pp. (1994).

H_2
VUV Emission Spectrum
Wavelengths
Assignments
78.6-171.4 nm
Tables

77960. Tso, H.C.W., D.J.W. Geldart and P. Chylek, "Anharmonicity and Cross Section for Absorption of Radiation by Water Dimer," *J. Chem. Phys.* 108, 5319-5329 (1998).

$(H_2O)_2$
Absorption
Cross Sections
Overtone Contributions
Calculations

77961.	Hishikawa, A., H. Sato and K. Yamanouchi, "Ω-Type Doubling Reversal in the $B^3\Pi_1$ State of ^{200}HgAr as a Probe of the Long-Range Potential of the $A^3\Pi_{0+}$ State," *J. Chem. Phys.* 108, 9202-9205 (1998).	HgAr(B-X) 2-Color REMPI Mass Analysis Perturbing A-State Vibrational Levels
77962.	Amano, K., K. Ohmori, T. Kurosawa, H. Chiba, M. Okunishi, K. Ueda, Y. Sato, A.Z. Devdariani and E.E. Nikitin, "(c←X) Laser Excitation Spectrum of the Hg-Ar van der Waals Complex," *J. Chem. Phys.* 108, 8110-8113 (1998).	HgAr(c-X) Pump/Probe Spectrum Constants D_0',D_0''
(78156)	Product Infrared/Ultraviolet Spectra, Matrix Study	$Hg(CH_3)_2 + h\nu$
77963.	Uehara, H., K. Horiai and T. Konno, "Analysis of Vibration-Rotational Spectra of KH," *J. Mol. Struct.* 413/414, 457-462 (1997).	KH(X) Dunham Constants Spectral Data Set
77964.	Jastrzebski, W., and P. Kowalczyk, "High Resolution Study of the ($B^1\Pi$-$X^1\Sigma^+$) Band System of KLi and the Isotopic Effect," *Spectrochim. Acta A. Mol. Spectrosc.* 54, 459-463 (1998).	KLi(B-X) Polarization Spectrum Dunham Constants
77965.	Little, A.M., G.K. Corlett and A.M. Ellis, "Ultraviolet Absorption of LiO in a Supersonic Jet," *Chem. Phys. Lett.* 286, 439-445 (1998).	LiO(C-X) LIF Spectrum Radiative Lifetime Li/N_2O Formation Method Comparisons
77966.	Lett, P.D., P.S. Julienne and W.D. Phillips, "Photoassociative Spectroscopy of Laser Cooled Atoms," *Ann. Rev. Phys. Chem.* 46, 423-452 (1995).	Li_2,Na_2 Photoassociation Spectra Laser Cooling Methods Review
77967.	Higgins, J., C. Callegari, J. Reho, F. Stienkemeier, W.E. Ernst, M. Gutowski and G. Scoles, "Helium Cluster Isolation Spectroscopy of Alkali Dimers in the Triplet Manifold," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4952-4965 (1998).	Li_2,Na_2,K_2,NaK Triplet States LIF Spectra He_n Cluster Attachment Method P.E. Curves
77968.	Fletcher, D.A., K.Y. Jung and T.C. Steimle, "Erratum - Molecular Beam Optical Stark Spectroscopy of MoN [*J. Chem. Phys.* 99, 901-905 (1993)]," *ibid.* 108, 10327 (1998).	MoN(A,X) Stark Spectra Dipole Moments Erratum

77969.	Kobayashi, K., and S. Saito, "The Microwave Spectrum of the NF Radical in the Second Electronically Excited ($b^1\Sigma^+$) State: Potentials of the Three Low-lying States ($X^3\Sigma^-$,$a^1\Delta$,$b^1\Sigma^+$)," *J. Chem. Phys.* 108, 6606-6610 (1998).	NF(b,a) Microwave Spectra Rotational Constants
77970.	Pratt, S.T., "Vibrational Autoionization and Predissociation in High Rydberg States of Nitric Oxide," *J. Chem. Phys.* 108, 7131-7140 (1998).	NO Rydberg States Autoionization Predissociation Channels State Mixing
77971.	Shafizadeh, N., P. Brechignac, M. Dyndgaard, J.H. Fillion, D. Gauyacq, B. Levy, J.C. Miller, T. Pino and M. Raoult, "A, C and D Electronic States of the Ar-NO van der Waals Molecule Revisited: Experiment and Theory," *J. Chem. Phys.* 108, 9313-9326 (1998).	NO.Ar(D,C,A-X) LIF/REMPI Spectra Measurements Theoretical Interpretations
77972.	Bush, A.M., J.M. Dyke, P. Mack, D.M. Smith and T.G. Wright, "Production of Rg^+ Ions in the Resonance-Enhanced Multiphoton Ionization Spectroscopy of Rg.NO(Rg=Ar,Kr and Xe)," *Chem. Phys.* 223, 239-249 (1997).	NO.Ar;NO.Kr NO.Xe REMPI Spectra Rg^+ Formation
77973.	Brandi, R., F. Santoro and C. Petrongolo, "Ab Initio Study of NO_2. VII. ($A^2B_2 \leftarrow X^2A_1$) Nonadiabatic Franck-Condon Absorption Spectrum," *Chem. Phys.* 225, 55-62 (1997).	NO_2(A-X) Absorption Spectrum Intensities Calculations
77974.	Lievin, J., A. Delon and R. Jost, "Absorption Cross Section of NO_2 by the Reflection Method from ab Initio Calculations Involving the Three Low-lying Electronic States," *J. Chem. Phys.* 108, 8931-8943 (1998).	NO_2(B,A-X) Absorption Cross Sections P.E. Surfaces Calculations
77975.	Shibuya, K., C. Terauchi, M. Sugawara, K. Aoki, K. Tsuji and S. Tsuchiya, "Vibrational Level Structure of $NO_2(C^2A_2)$ in the Energy Region of 16200-21000 cm^{-1}: Evidence for the Breakdown of C_{2v} Symmetry," *J. Mol. Struct.* 413/414, 501-509 (1997).	NO_2(C) Vibrational Level Structure (D-C) Fluorescence Analysis Symmetry
77976.	Krim, L., and N. Lacome, "The NO Dimer, ^{14}N and ^{15}N Isotopomers Isolated in Argon Matrix: A Near-, Mid- and Far-Infrared Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2289-2296 (1998).	$(NO)_2$ FTIR Spectra Fundamentals/ Overtone Bands Frequencies Isotopomers Matrix Study

77977. Grantier, D.R., and J.L. Gole, "Raman-Like Pumping from Long Range Excited Alkali Atom-Alkali Dimer Interactions," *Chem. Phys.* 223, 259-272 (1997). — Na_2(B,A-X); RRS Spectrum; Na(^2P_J) Emission; Pumping

77978. de Vivie-Riedle, R., J. Gaus, V. Bonacic-Koutecky, J. Manz, B. Reischl-Lenz and P. Saalfrank, "Theoretical Study of the Absorption Spectrum of the Pseudorotating Na_3(B)," *Chem. Phys.* 223, 1-14 (1997). — Na_3(B-X); Absorption; P.E. Surfaces; Synthetic Spectrum; Calculations

(78158) Photodetachment Spectrum Calculations — $OHCl^-$

77979. Naus, H., A. de Lang and W. Ubachs, "($b^1\Sigma_g^+$-$X^3\Sigma_g^-$),(0,0) Band of Oxygen Isotopomers in Relation to Tests of the Symmetrization Postulate in $^{16}O_2$," *Phys. Rev. A: At. Mol. Opt. Phys.* 56, 4755-4763 (1997). — O_2(b-X),(0,0); Cavity Ringdown; Spectrum; Constants; Isotopomers

77980. Tanaka, T., H. Yoshii, Y. Morioka, T. Hayaishi, K. Ito and R.I. Hall, "High Resolution Threshold Photoelectron Spectra of Molecular Oxygen in the 18-24 eV Region," *J. Chem. Phys.* 108, 6240-6248 (1998). — O_2^+; 9 Electronic States; Assignments; Constants; Photoelectron Spectra

77981. Palm, H., and F. Merkt, "Role of Electron Spin Coupling in Molecular Photoionization: The ($b^4\Sigma_g^- \leftarrow X^3\Sigma_g^-$) Photoelectronic Transition of O_2," *Phys. Rev. Lett.* 81, 1385-1388 (1998). — O_2^+(b)-O_2(X); ZEKE/PES; Spectrum; Transition; Propensities

77982. Bacis, R., A.J. Bouvier and J.M. Flaud, "The Ozone Molecule: Electronic Spectroscopy," *Spectrochim. Acta A. Mol. Spectrosc.* 54, 17-34 (1998). — O_3; Low-lying; Excited States; Absorption; Spectra; Review

77983. Gunther, J., S.M. Anderson, G. Hilpert and K. Mauersberger, "Rotational Structure in the Absorption Spectra of $^{18}O_3$ and $^{16}O_3$ Near 1 μm: A Comparative Study of the $^3A_2$ and $^3B_2$ States," *J. Chem. Phys.* 108, 5449-5457 (1998). — O_3; $^{18}O_3$; 1 μm Absorption; High Resolution; Spectra; Assignments; Constants

77984. Johnson, B.R., B.-Y. Chuang, C.-W. Hsiao, L. Le and J.L. Kinsey, "Temperature Dependence and Dynamical Instability in the Hartley Absorption System of Ozone," *J. Chem. Phys.* 108, 7670-7678 (1998). — O_3; Hartley Absorption; Spectrum; Weak Oscillations; T Dependence; Dynamics

77985. Tsai, C.C., R.S. Freeland, J.M. Vogels, H.M.J.M. Boesten, B.J. Verhaar and D.J. Heinzen, "Two-Color Photoassociation Spectroscopy of Ground State Rb_2," *Phys. Rev. Lett.* 79, 1245-1248 (1997).

Rb_2
12 Vibrational
Near Limit Levels
2-Color
Photoassociation
Spectroscopy

(78398) Photoionization Spectra, IPS, Discharged Cl_2/H_2S

SCl_2,HSCl,S_2Cl
S_2,S_3,HS_2Cl
H_2S_2,H_2S_3

77986. Civis, S., A. Walters, M.Yu. Tretyakov, S. Bailleux and M. Bogey, "Submillimeter-Wave Spectral Lines of Negative Ions (SH^- and SD^-) Identified by their Doppler Shift," *J. Chem. Phys.* 108, 8369-8373 (1998).

SD^-,SH^-
Submillimeter Wave
Spectra
Velocity
Modulation
Constants

77987. Wienkoop, M., P. Murtz, P.-C. Schumann, M. Havenith and W. Urban, "First Observation of Rovibrational Transitions of the SiC Radical by Infrared LMR Spectroscopy," *Chem. Phys.* 225, 17-21 (1997).

SiC(X),(1,0)
LMR Spectrum
Band Origin

77988. Tanaka, T., M. Tamura and K. Tanaka, "Infrared Diode Laser Spectroscopy of the SiF Radical: Analysis of Hot Bands up to ν=9-8," *J. Mol. Struct.* 413/414, 153-166 (1997).

SiF(X,v≤9)
IR Spectra
Diode Laser
Constants

77989. Fujitake, M., and E. Hirota, "Detection of a New Halosilylene, SiFCl, by Microwave Spectroscopy," *J. Mol. Struct.* 413/414, 21-30 (1997).

SiFCl
Rotational
Spectrum
Structure
Frequencies

77990. Izuha, M., S. Yamamoto and S. Saito, "Microwave Spectrum of HSiO in the X^2A' Ground Electronic State," *J. Mol. Struct.* 413/414, 527-535 (1997).

HSiO(X)
Rotational
Spectrum
Constants
Structure

77991. Brown, F.X., S. Yamamoto and S. Saito, "The Microwave Spectrum of the HSiS Radical in the $^2A'$ Ground Electronic State," *J. Mol. Struct.* 413/414, 537-544 (1997).

SiHS(X)
Microwave
Spectrum
Constants
Structure

77992. Escribano, R., and A. Campargue, "Absorption Spectroscopy of SiH_2 Near 640 nm," *J. Chem. Phys.* 108, 6249-6257 (1998).

SiH_2(A-X)
Intracavity
Absorption
Spectrum
Structure
Constants

77993. Xu, C., T.R. Taylor, G.R. Burton and D.M. Neumark, "Photoelectron Spectroscopy of Si_nH^- (n=2-4) Anions," *J. Chem. Phys.* 108, 7645-7652 (1998).

Si_nH,n=2-4
Photoelectron Spectra
Frequencies
EAs

77994. Kushto, G.P., P.F. Souter and L. Andrews, "An Infrared Spectroscopic and Quasirelativistic Theoretical Study of the Coordination and Activation of Dinitrogen by Thorium and Uranium Atoms," *J. Chem. Phys.* 108, 7121-7130 (1998).

ThN,ThN_2
UN,UN_2
Laser Ablation
Th,U/N_2
FTIR Analysis
Matrix Study

77995. Wu, H., and L.-S. Wang, "A Photoelectron Spectroscopic Study of Monovanadium Oxide Anions (VO_x^-, x=1-4)," *J. Chem. Phys.* 108, 5310-5318 (1998).

VO_n,v=1-4
Photoelectron Spectra
Low-lying States
Constants,Energies
EAs

77996. Liu, S., A. Hishikawa and K. Yamanouchi, "Mass-Resolved Vacuum Ultraviolet Laser Spectroscopy of XeAr: Two Competing Predissociation Pathways in the C1 State," *J. Chem. Phys.* 108, 5330-5337 (1998).

XeAr(C-X)
Absorption Spectrum
Constants
Predissociation Mechanisms

27. EXCITED STATE LIFETIMES/QUENCHING

77997. Zagrebin, A.L., and M.G. Lednev, "Radiative Decay of the (nsnp$^3P_2$) State in Cd*, Ba*, Yb*, Hg*+He Thermal Collisions," *Opt. Spectrosc., Russia* 83, 196-200 (1997).

M*($^3P_2$)+He
M=Ba,Cd,Hg,Yb
Collision Induced Radiative Decay
Rate Constants

77998. Le Picard, S.D., B. Bussery-Honvault, C. Rebrion-Rowe, P. Honvault, A. Canosa, J.M. Launay and B.R. Rowe, "Fine Structure Relaxation of Aluminum by Atomic Argon Between 30 and 300 K: An Experimental and Theoretical Study," *J. Chem. Phys.* 108, 10319-10326 (1998).

Al($^2P_{1/2,3/2}$)+Ar
Fine Structure Relaxation
Rate Constants

77999. Reignier, D., T. Stoecklin, S.D. Le Picard, A. Canosa and B.R. Rowe, "Rate Constant Calculations for Atom-Diatom Reaction Involving an Open-Shell Atom and a Molecule in a Σ Electronic State: Application to the Reaction Al($^2P_{1/2,3/2}$)+O_2($X^3\Sigma_g^-$)$\rightarrow$AlO($X^2\Sigma^+$)+ O($^3P_{2,1,0}$)," *J. Chem. Soc., Faraday Trans.* 94, 1681-1686 (1998).

Al($^2P_{1/2,3/2}$)+O_2
Rate Constants
T Dependence
Spin-Orbit Effects
Calculations

78000. Husain, D., J. Geng, J. Lei, F. Castano and M.N.S. Rayo, "Chemiluminescence from the Reactions of Ba[6s5d(^3D_J)] with CF_3Br and CF_2Br_2 Including Branching Ratios into the Electronic States BaBr($A^2\Pi_{1/2}$,$A^2\Pi_{3/2}$,$B^2\Sigma^+$) Following the Pulsed Dye Laser Excitation of Atomic Barium," *Combust. Flame* 113, 566-578 (1998).

Ba(^3D_J)+CF_2Br_2
Ba(^3D_J)+CF_3Br
BaBr(B,A-X)
Chemiluminescence
Branching Ratios

78001.	Husain, D., J. Lei, F. Castano and M.N.S. Rayo, "Investigation of Branching Ratios into BaI($A^2\Pi_{1/2,3/2}$,$B^2\Sigma^+$) from the Reaction of Ba[6s5d(^3D_J)] with CH_3I by Time-Resolved Atomic Emission and Molecular Chemiluminescence Following Pulsed Dye Laser Excitation of Atomic Barium," *Z. Phys. Chem. (Munchen)* 203, 95-111 (1998).	Ba(^3D_J)+CH_3I Quenching BaI(B,A) Product Branching Ratios
78002.	Berg, L.-E., N. Gador, D. Husain, H. Ludwigs and P. Royen, "Lifetime Measurements of the $A^2\Pi_{1/2}$ State of BaF using Laser Spectroscopy," *Chem. Phys. Lett.* 287, 89-93 (1998).	BaF(A) Radiative Lifetime Measurement
(78277)	Lifetimes, P.E. Curves, Low-lying States, Spectral Constants, Transition Probabilities, Calculations	BiN*
78003.	Martin, M., and C. Cerezo, "Collisional Removal of CD($A^2\Delta$ and $B^2\Sigma^-$) by Xe: Dependence on Rotational and Vibrational Excitation," *Chem. Phys. Lett.* 288, 799-803 (1998).	CD(B,A)+Xe Quenching Rate Constants v,N Dependences
78004.	Chen, C., F. Wang, Y. Chen and X. Ma, "Temperature Effect on Quenching of CH($A^2\Delta$)," *Chem. Phys.* 230, 317-325 (1998).	CH(A)+M Quenching Rate Constants T Dependences M=C_2H_4,O_2, C_2-C_4 Alcohols, C_5-C_7 Alkanes
78005.	Tamura, M., P.A. Berg, J.E. Harrington, J. Luque, J.B. Jeffries, G.P. Smith and D.R. Crosley, "Collisional Quenching of CH(A), OH(A) and NO(A) in Low Pressure Hydrocarbon Flames," *Combust. Flame* 114, 502-514 (1998).	CH(A),NO(A),OH(A) Lifetimes Quenching Rates Low Pressure CH_4/Air
(78166)	Lifetime, Dissociation Product Velocities, Br/Br* Branching, Ion Imaging Monitor	CH_3Br(A)
78006.	Cacciani, P., W. Ubachs, P.C. Hinnen, C. Lynga, A. L'Huillier and C.-G. Wahlstrom, "Lifetime Measurements of the $E^1\Pi$(v=0,1) States of $^{12}C^{16}O$, $^{13}C^{16}O$ and $^{13}C^{18}O$," *Astrophys. J.* 499, L223-L226 (1998).	CO(E,v=0,1) Radiative Lifetimes Isotope Effects
(77931)	Radiative Lifetimes, (a′-X) Absorption, a′/A State Mixing, Field Effects	CO(a′),v=14,N
(77796)	Quenching Rate Constant	CO(a)+CO_2
(78355)	E-E Transfer, NO(B,A,a) Product Channels, Cross Sections	CO(a)+NO
78007.	Farley, D.R., and R.J. Cattolica, "Collisional Quenching and Excitation Cross Sections of the CO_2^+ $A^2\Pi$(1→3,0,0) and $B^2\Sigma^+$ (0,0,0) Excited States from Electron Impact Ionization," *Chem. Phys. Lett.* 274, 445-450 (1997).	CO_2^+(B,A)+M Quenching Rate Constants M=CO_2
(78249)	Quenching Rate Constants, CO/He Discharge, C_2 Formation	C_2(d,A)+CO,He

(77940)	Lifetime, (a,A-X) LIF, Phosphorescence, Matrix Study	$C_3(A)$
(77941)	Lifetimes, (B-X) LIF, Isomers	$CH_2COCH_3(B)$
(78354)	Aromatics, Review	E-V Relaxation
78008.	Barsotti, S., F. Fuso, A.F. Molisch and M. Allegrini, "Cross Section Measurement for the Energy Pooling Collisions: $Cd(5p^3P_1)+Cd(5p^3P_1)\rightarrow Cd(5d^3D_J)+Cd(5s^1S_0)$," *Phys. Rev. A: At. Mol. Opt. Phys.* 57, 1778-1786 (1998).	$Cd(^3P_1)+Cd(^3P_1)$ Energy Pooling Cross Sections
78009.	Chang, L.-C., Y.-S. Hwang and T.-M. Su, "Recombination Reactions of Atomic Chlorine in Inert Gases: A Vibrationally Resolved Transient Kinetics Study at Pressures Below 1 atm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3711-3718 (1998).	$Cl_2(B,A,v)+M$ Quenching Rate Constants $Cl+Cl+M$ Kinetic Model Energy Relaxation
78010.	Mullman, K.L., J.C. Cooper and J.E. Lawler, "Radiative Lifetimes and Ultraviolet Branching Fractions for Resonance Lines of Co^+," *Astrophys. J.* 495, 503-507 (1998).	Co^+ Radiative Lifetimes Branching Ratios 28 f-Values Measurements
78011.	Haynes, C.L., and K. Honma, "Kinetics of Excited-State $Cr(a^5D_J, a^5S_2)$ Depletion by O_2, NO and N_2," *J. Chem. Soc., Faraday Trans.* 94, 1171-1177 (1998).	$Cr(^5D_J)+NO,N_2,O_2$ $Cr(^5S_2)+NO,N_2,O_2$ Rate Constants
78012.	Lintz, M., and M.A. Bouchiat, "Dimer Destruction in Cs Vapor by a Laser Close to Atomic Resonance," *Phys. Rev. Lett.* 80, 2570-2573 (1998).	$Cs(^2P)+Cs_2$ Dimer Dissociation Cross Sections Laser Induced Atomic Absorption Method
78013.	Lee, K., H.S. Son, S.C. Bae and J.K. Ku, "Collisional Quenching of Ga(5p) Atoms by H_2, D_2 and CH_4," *Chem. Phys. Lett.* 288, 531-537 (1998).	$Ga(5p^2P_{3/2})+M$ $Ga(5s^2S_{1/2})+M$ Quenching Cross Sections $M=CH_4,H_2,D_2$ Branching Ratios
78014.	Husain, D., A.X. Ioannou and M. Kabir, "Collisional Quenching of Electronically Excited Germanium Atoms, $Ge(4p^2(^1S_0))$, by Small Molecules Investigated by Time-Resolved Atomic Resonance Absorption Spectroscopy," *J. Photochem. Photobiol. A. Chem.* 110, 213-220 (1997).	$Ge(^1S_0)+M$ Quenching Rate Constants 13 Collision Partners

78015. Husain, D., A.X. Ioannou and M. Kabir, "The Collisional Quenching of Electronically Excited Germanium Atoms, $Ge[4p^2(^1S_0)]$, with Olefins and Acetylenes Investigated by Time-Resolved Atomic Resonance Absorption Spectroscopy," *Z. Phys. Chem. (Munchen)* 203, 213-230 (1998).

$Ge(^1S_0)+RH$
RH=17 Alkenes, 10 Alkynes
Quenching
Rate Constants

78016. Ter-Avetisyan, S.A., and V.O. Papanyan, "Afterglow of Resonantly Excited Cesium Ions in a He-Cs Mixture," *Opt. Spectrosc., Russia* 82, 696-700 (1997).

$He(^{1,3}S)+Cs$
Penning Ionization
$He^+ + He + He$
Cross Sections
$He(^3S)/Cs$
Diffusion Coefficient

78017. Vojtik, J., R. Kotal and J. Fiser, "Classical Trajectory Picture of the Autoionization Event in $He(2^3S)$-D_2 Penning Ionization: Collision Energy Dependence," *Chem. Phys.* 229, 165-174 (1998).

$He(2^3S)+D_2$
Penning Ionization
Reaction Dynamics
Electron Energies
$D_2^+(v)$ Product

78018. Ishida, T., "Quantum-Chemical and Classical-Dynamics Calculations for Penning Ionization $H_2O + He(2^1S) \rightarrow H_2O^+ + He + e^-$: Comparison with the Metastable $He(2^3S)$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2283-2288 (1998).

$He(2^1S)+H_2O$
Penning Ionization
H_2O^+ Product
Entrance Channel
P.E. Surface
Dynamics

78019. Kishimoto, N., M. Furuhashi and K. Ohno, "Two-Dimensional Penning Ionization Electron Spectrum of N_2 by Collision with He (2^3S) Metastable Atoms," *J. Electron Spectrosc. Relat. Phenom.* 88-91, 143-147 (1998).

$He(2^3S)+N_2$
Penning Ionization
$N_2^+(B,A,X)$ Product
Branching Ratios
Cross Sections

78020. Kartoshkin, V.A., and G.V. Klement'ev, "Chemi-ionization and Spin Exchange in Collisions of Polarized Atoms with Paramagnetic Molecules. II. Calculations of the Spin-Exchange, Magnetic Resonance Frequency Shift, and Chemi-ionization Cross Sections for the $He(2^3S_1)$-$O_2(^3\Sigma_g^-)$ System," *Opt. Spectrosc., Russia* 80, 545-550 (1996).

$He(2^3S_1)+O_2$
Penning Ionization
Spin Exchange
Cross Sections
Calculations

78021. Kryukov, N.A., P.A. Savel'ev and M.A. Chaplygin, "Radiative-Collisional Quenching of Metastable Mercury Atoms by Krypton," *Opt. Spectrosc., Russia* 82¸ 691-695 (1997).

$Hg(^3P_2)+Kr$
Quenching
Rate Constant

(78363) Vibrational Relaxation, Rotational Energy Effects, Transition Probability Functions

HgBr(B,v)+Rg

78022. Figen, Z.G., H.C. Tran and J.G. Eden, "Collisional Quenching of Hg_2 $(A0_g^+)$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4972-4975 (1998).

$Hg_2(A)+Hg$
$Hg_2(A)+Hg+Hg$
Rate Constants
LIF Monitor

78023. Kireev, S.V., and S.L. Shnyrev, "Buffer Gas Quenching of the $^{127}I_2$ Fluorescence Excited by He-Ne Laser Radiation at 633 nm," *Opt. Spectrosc., Russia* 83, 351-353 (1997). — $I_2(B)+M$ Quenching Rate Constants M=7 Colliders LIF

78024. Kireev, S.V., and S.L. Shnyrev, "Laser Induced Fluorescence Detection of $^{127}I_2$ and $^{129}I_2$ Iodine Isotopes in Various Gases," *Opt. Spectrosc., Russia* 81, 326-329 (1996). — I_2(B-X) LIF(633 nm) CO_2,N_2,O_2,Air Quench Effects Isotopic Monitoring

78025. Buchachenko, A.A., "Predissociation of the Rg.I_2(B) (Rg=Ne,Ar,Kr) Complexes: Simulations Based on the First Order Diatomics-in-Molecule Perturbation Theory," *Chem. Phys. Lett.* 292, 273-281 (1998). — I_2(B).Rg Predissociation Rate Constants Rg=Ne,Ar,Kr I_2(B,v) Products Calculations

78026. De Filippo, G., S. Guldberg-Kjaer, S. Milosevic, J.O.P. Pedersen and M. Allegrini, "Reverse Energy Pooling in a K-Na Mixture," *Phys. Rev. A: At. Mol. Opt. Phys.* 57, 255-266 (1998). — $K(5^2D)+Na$ $K(7^2S)+Na$ Reverse Energy Pooling Rate Constants

(77965) Radiative Lifetimes, (C-X) LIF Spectrum, Li/N_2O Formation Method Comparisons — LiO(C)

(78173) Quenching Dynamics, MgH(v=0,1,N) Product State Distributions — $Mg(^1P_1)+CH_4$

78027. Lotz, C., and F. Stuhl, "Quenching of NH/ND($b^1\Sigma^+$) by H_2, D_2 and N_2 at Different Temperatures and Pressures," *J. Chem. Soc., Faraday Trans.* 94, 823-826 (1998). — NH(b)+H_2,D_2,N_2 ND(b)+H_2,D_2,N_2 Quenching Rate Constants T Dependence Pressure Effects

(78174) Quenching Rate Constants, M=N_2,N_2O, O_2,O_3, Measurements — NO(B,v=0-3)+M

(77970) Predissociation/Autoionization Channels, State Mixing — NO Rydberg States

(77807) Dissociative Recombination, Product Branching Ratios, Comparisons — $N_2^+(A,X)+e^-$

78028. Motzkus, M., G. Pichler, K.L. Kompa and P. Hering, "Vibrationally Induced Formation of NaH in the Na(3p)+H_2 Collision System: Rate Equation Model and Comparison with Experimental Results," *J. Chem. Phys.* 108, 9291-9300 (1998). — $Na(^2P_J)+H_2$ Quenching Product H_2(v) Role

78029. Saha, B.C., "Quenching of Na(4p) by He and H_2: A Molecular State Treatment," *Phys. Rev. A: At. Mol. Opt. Phys.* 56, 2909-2912 (1997). — $Na(^2P)$+He,H_2 Quenching Cross Sections Model

(78272) Predissociative Vibrational Levels, P.E. Curve, OODR Measurements | $Na_2(4^3\Sigma_g^+)$

78030. Vajda, S., S. Rutz, J. Heufelder, P. Rosendo, H. Ruppe, P. Wetzel and L. Woste, "Observation of Predissociated Excited States in Mixed Alkali Trimer Clusters Na_2K and K_2Na: Time-Resolved Spectroscopy of Bound-Free Transitions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4066-4068 (1998).
Na_2K,K_2Na
Excited State
Predissociation
fs Pump/Probe

78031. Lescop, B., M.B. Arfa, M. Cherid, G. Le Coz, G. Sinou, G. Fanjoux, A. Le Nadan and F. Tuffin, "Penning Ionization Electron Spectroscopy of the C_2H_2 Molecule by $Ne^*(3^3P_2,3^3P_0)$ Metastable Atoms," *J. Electron Spectrosc. Relat. Phenom.* 87, 51-59 (1997).
$Ne(^3P_{2,0})+C_2H_2$
Penning Ionization
Product $C_2H_2^+(v)$
Electron
Angular
Distributions

78032. Lugez, C.L., K.K. Irikura and M.E. Jacox, "Experimental and ab Initio Study of the Infrared Spectra of Ionic Species Derived from PF_5, PF_3 and F_3PO and Trapped in Solid Neon," *J. Chem. Phys.* 108, 8381-8393 (1998).
Ne^*+PF_3,PF_5
Product Ions
FTIR Spectra
Assignments
Frequencies
Matrix Study

78033. Lugez, C.L., M.E. Jacox, R.A. King and H.F. Schaefer III, "Experimental and ab Initio Study of the Infrared Spectra of Ionic Species Derived from SF_6 and SF_4 and Trapped in Solid Neon," *J. Chem. Phys.* 108, 9639-9650 (1998).
Ne^*+SF_4,SF_6
Penning Ionization
FTIR Spectra
Frozen Products
Matrix Trapping

(78288) Predissociation Lifetimes, Interactions, P.E. Curves, Calculations
NeH,NeD
Rydberg States

78034. Cronkhite, J.M., and P.H. Wine, "Branching Ratios for BrO Production from Reactions of $O(^1D)$ with HBr, CF_3Br, CH_3Br, CF_3ClBr and CF_2HBr," *Int. J. Chem. Kinet.* 30, 555-563 (1998).
$O(^1D)+CF_2ClBr$
$O(^1D)+CF_2HBr$
$O(^1D)+CF_3Br,CH_3Br$
$O(^1D)+HBr$
BrO Product
Yields

78035. Sorokin, V.I., N.P. Gritsan and A.I. Chichinin, "Collisions of $O(^1D)$ with HF, F_2, XeF_2, NF_3 and CF_4: Deactivation and Reaction," *J. Chem. Phys.* 108, 8995-9003 (1998).
$O(^1D)+CF_4,HF,F_2$
$O(^1D)+NF_3,XeF_2$
Quenching/
Reaction Channel
Cross Sections
Measurements

78036. Brownsword, R.A., M. Hillenkamp, P. Schmiechen, H.-R. Volpp and H.P. Upadhyaya, "Absolute Reactive Cross Section for H Atom Formation in the Reaction of Translationally Energetic $O(^1D)$ Atoms with Methane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4438-4443 (1998).
'Hot' $O(^1D)+CH_4$
37 kJ mol^{-1} Energy
Cross Section
H Product Channel

(78179) $OH(v=0,1,J)$ Product Distributions, Comparisons, Cluster Effects
$O(^1D)+CH_4,C_2H_6,C_3H_8$
$N_2O.RH+h\nu$

(78178) OH(J) Product Energy Distributions, Cluster Effects | $O(^1D) + HCl.Ar$
 $O + HCl.Ar$

(78178)	OH(J) Product Energy Distributions, Cluster Effects	$O(^1D) + HCl.Ar$ $O + HCl.Ar$
(78180)	OH,OD Product Velocity Distributions, Crossed Beams Mechanism	$O(^1D) + H_2, D_2$
(78174)	NO(X,v=11-17) Product State Distributions, Measurements	$O(^1D) + N_2O$
(78242)	Reaction Dynamics, Channels, Transition State Energies, Calculations	$O_2(a) + C_2H_3OH$
78037.	Kukueva, V.V., "Change of Intensity of ($a^1\Delta_g \rightarrow X^3\Sigma_g^-$) Transition in Oxygen Molecule Upon Interaction with H_2, N_2 and CS_2," *Theor. Exp. Chem., Russia* 32, 125-128 (1996).	$O_2(a) + Cl_2$ $O_2(a) + H_2, N_2$ Radiative Transition Probability Enhancements Collision Complexes Calculations
78038.	Kobzev, G.I., B.F. Minaev, Z.M. Muldakhmetov, S.N. Martynov, S.A. Beznosyuk and T.I. Mozgovaya, "Mechanism of Enhancement of the ($a^1\Delta_g$-$b^1\Sigma_g^+$) Transition in the Oxygen Molecule Caused by Intermolecular Interaction," *Opt. Spectrosc., Russia* 83, 58-62 (1997).	$O_2(a) + H_2$ Collisional (a-b),(a-X) Transition Probability Enhancements Modeling
(77875)	Potential NO_x Formation Channel, Atmospheric Implications	$O_2(B) + N_2$
78039.	Li, Y., G. Hirsch and R.J. Buenker, "Theoretical Treatment of Predissociation of the (4pσ) $^{1,3}\Pi_u$ Rovibrational Levels in the Spectrum of the Oxygen Molecule," *J. Chem. Phys.* 108, 8123-8129 (1998).	$O_2(^{1,3}\Pi_u, ^1\Delta_u)$ Low-lying States Predissociation Linewidths State Interaction Mechanisms
78040.	Berzinsh, U., S. Svanberg and E. Biemont, "Radiative Lifetimes for the 4p Excited States of Phosphorus and the Oscillator Strengths of Solar Lines," *Astron. Astrophys.* 326, 412-416 (1997).	P(4p) Radiative Lifetimes 6 Levels Oscillator Strengths
78041.	Tayal, S.S., "Oscillator Strengths of Allowed and Intercombination Transitions in Neutral Sulfur," *Astrophys. J.* 497, 493-497 (1998).	S Radiative Lifetimes f-Values Calculations
78042.	Biemont, E., H.P. Garnir, S.R. Federman, Z.S. Li and S. Svanberg, "Lifetimes and Oscillator Strengths for Ultraviolet Transitions in Neutral Sulfur," *Astrophys. J.* 502, 1010-1014 (1998).	S Radiative Lifetimes Low-lying States f-Values

78043. Wheeler, M.D., S.M. Newman and A.J. Orr-Ewing, "Predissociation of the $B^3\Sigma_u^-$ State of S_2," *J. Chem. Phys.* 108, 6594-6605 (1998).

S_2(B,v=10-22)
Predissociation
Cavity Ringdown
Linewidths
Mechanisms

(78291) P.E. Curves, Low-lying States, Lifetimes, Spectral Constants, Spin-Orbit Splittings, Calculations

SbH*

78044. McKendrick, K.G., "What Determines the Disposal of Energy in the Products of Electronically Inelastic Collisions? A Comparative Case Study of SiCl and SiF," *J. Chem. Soc., Faraday Trans.* 94, 1921-1932 (1998).

$SiCl(^2\Delta)+M$
$SiF(^2\Delta)+M$
Quenching
Energy Transfers
Branching Ratios
Review

78045. Jackson, N.A., C.J. Randall and K.G. McKendrick, "Polarization Effects in Electronically Inelastic Collisions: $SiF(C^2\Delta)+H_2\rightarrow SiF(B^2\Sigma^+)+H_2$," *Chem. Phys.* 233, 45-55 (1998).

$SiF(C)+H_2$
Quenching
(C-B) Relaxation
Polarization
Effects

78046. Neuman, J.A., and A. Gallagher, "Effects of Alignment on Strontium Energy Pooling Collisions," *Phys. Rev. A: At. Mol. Opt. Phys.* 57, 2231-2234 (1998).

$Sr(^3P_1)+Sr(^3P_1)$
Energy Pooling
Rate Constants
Channels
Alignment Effects

(77996) Predissociation Mechanisms, Absorption Spectrum, Constants

XeAr(C)

(78365) Vibrational Relaxation Channels

XeF(B,C)+Rg

28. FRANCK-CONDON FACTORS/TRANSITION PROBABILITIES

(See also Section 27 for Lifetimes and Transition Probabilities)

(78274) Ten Cases, P.E. Curves, Long Range Free/Bound F.C. Factors

Mixed Alkali Dimers

(77956) Oscillator Strengths, Overtone Transitions, Measurements

$HNO_3(3,4\nu_{OH})$

78047. Astashkevich, S.A., N.V. Kokina and B.P. Lavrov, "Branching Ratios in v″ Progressions of the ($I^1\Pi_g^-$, v′$\rightarrow B^1\Sigma_u^+$,v″) Bands of the H_2 Molecule," *Opt. Spectrosc., Russia* 83, 679-684 (1997).

H_2(I-B)
v′=0-3,v″=0-8
Transition
Probabilities
FC Discrepancies

78048. Hattig, C., O. Christiansen and P. Jorgensen, "Coupled Cluster Response Calculations of Two-Photon Transition Probability Rate Constants for Helium, Neon and Argon," *J. Chem. Phys.* 108, 8355-8359 (1998).

He,Ne,Ar+2hν
Transition
Probabilities
Low-lying States
Calculations

78049.	Gamalii, V.F., "Measurement of the Oscillator Strength of the ($4^2P_{3/2}$-$6^2S_{1/2}$) Transition in Atomic Potassium by the Intracavity Laser Technique," *Opt. Spectrosc., Russia* 83, 662-663 (1997).	$K(4^2P_{3/2}$-$6^2S_{1/2})$ Oscillator Strength Intracavity Absorption
78050.	Ivanov, V.S., and V.B. Sovkov, "Analysis of Structural Continua of Bound-Free Electronic Transitions in Diatomic Molecules in the Inverse Perturbation Approximation: The Transition Electronic Moment," *Opt. Spectrosc., Russia* 83, 63-66 (1997).	$Li_2(2^3\Pi_g$-a) Bound/Free Spectra Transition Moment Determination Method
(77981)	Transition Propensities, ZEKE/PES Spectrum	O_2^+(b)-O_2(X)
78051.	Curry, J.J., and J.E. Lawler, "Branching Ratio for the ($^5S_2^0$-$^3P_{2,1}$) Inter-System Resonance Multiplet in P^+," *Astron. Astrophys.* 328, 752-755 (1997).	$P^+(^5S_2$-$^3P_{2,1})$ Emission Branching Ratio Measurement

29. LINESHAPES/STRENGTHS

(78304)	Infrared Intensities, Frequencies, Structural Calculations	CH_2(c,b,a,X)
(77927)	Line Intensities, Absorption Spectrum, D-Isotopes, Calculations	CH_2^+(A-X)
(78306)	Infrared Intensities, Frequencies, Structural Calculations	CH_2Cl_2
(78317)	Infrared Intensities, Frequencies, Structural Calculations, Sensitivity to Wave Function Modifications	$C_2H_2F_2$ $C_2H_2Cl_2$
(77943)	Infrared Band Intensities, FTIR Spectra, Assignments	C_4N_2
(78332)	Infrared Intensities, Geometries, Frequencies, Structural Calculations	FONO,ClONO,BrONO FNO_2,$ClNO_2$,$BrNO_2$
(78281)	Infrared Intensities, Dipole Moments, P.E. Surfaces, Calculations	HOBr HOCl
(78283)	Far Wing Collision Induced Absorptions, Rg=Ar,Kr,Xe, P.E. Curves	HgRg(c-X)
(78339)	Infrared Intensities, Geometries, Frequencies, Energies, Structural Calculations	NH_2^+(c,b,aX)
(77973)	Synthetic Absorption Spectrum, $\leq$22000 cm^{-1}, Intensities	NO_2(A-X)
78052.	Nefedov, A.P., V.A. Sinel'shikov, A.D. Usachev, M.A. Khomkin, N. Gerasimov, L. Zarkova, G. Paeva and P. Pirgov, "Measurement of the Reduced Absorption Coefficient in the Far Wings of Sodium D-Lines Broadened by Carbon Dioxide Molecules in a $C_2H_2/O_2/CO_2$ Flame," *Opt. Spectrosc., Russia* 83, 695-700 (1997).	Wing Lineshapes $Na(^2P_{1/2,3/2}$-$^2S_{1/2})$ C_2H_2/O_2 Flame CO_2,H_2O,N_2 Broadening Comparisons

(78176)	Doppler Profiles, Kinetic Energies, HOCl+hν	OH
78053.	Ray, B., and P.N. Ghosh, "Collisional Narrowing and Pressure Broadening of the Oxygen A-Band Transitions," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 537-543 (1997).	O_2(b-X) Linewidths Pressure Broadening Diode Laser Measurements
(78039)	Predissociative Linewidths, Low-lying States, Interaction Mechanisms	$O_2(^{1,3}\Pi_u, ^1\Delta_u)$
(78043)	Predissociative Linewidths, Cavity Ringdown Measurements, Mechanisms	S_2(B,v=10-22)
(78350)	Infrared Intensities, Structural Calculations, Geometries, Energies	SiH_2(B,A,a,X)

30. ANALYSIS/MONITORING TECHNIQUES

(See also Section 32 for Mapping and Tomographic Methods)

78054.	Trishenkov, M.A., *"Detection of Low Level Optical Signals: Photodetectors, Focal Plane Arrays and Systems,"* 8 Chapters, 458 pp., Kluwer Academic Publishers, Dordrecht, The Netherlands (1997).	Photodetectors CCD Arrays Optical Monitoring Monograph
78055.	Sneddon, J., "Sample Introduction in Atomic Spectroscopy," One of Five Reviews, 238 pp., Edited by J. Sneddon, in *Advances in Atomic Spectroscopy* 1, 81-124 (1992).	Atomic Analysis Spectroscopic Sample Introduction Methods Review
78056.	Croslyn, A.E., B.W. Smith and J.D. Winefordner, "A Review of Microwave Plasma Sources in Atomic Emission Spectrometry: Literature from 1985 to the Present," *Crit. Rev. Anal. Chem.* 27, 199-255 (1997).	Atomic Analysis Emission Microwave Plasmas Sensitivities Review
78057.	Pupyshev, A.A., V.N. Muzgin, N.L. Vasil'eva, T.K. Kostenko and E.K. Melnikova, "Thermodynamic Simulation of the Atomization of Elements in Acetylene/Air, Acetylene/Nitrous Oxide, Propane (Butane)/Nitrous Oxide and Methylacetylene/Air Flames," *J. Anal. Chem., Russia* 47, 1008-1020 (1992).	Atomic Analysis C_2H_2/N_2O,Air $C_3H_8, C_4H_{10}/N_2O$ CH_3CCH/Air 58 Elements Atomization Efficiencies
78058.	Li, K.-P., and J.D. Winefordner, "Analyte Excitation Mechanisms in the Inductively Coupled Plasma," One of Five Reviews, 238 pp., Edited by J. Sneddon, in *Advances in Atomic Spectroscopy* 1, 1-36 (1992).	ICP Atomic Analysis Excitation Mechanisms Review

78059. Simeonsson, J.B., M. Ezer, H.L. Pacquette, S.L. Preston and D.J. Swart, "Laser Induced Fluorescence of As, Se and Sb in the Inductively Coupled Plasma," *Spectrochim. Acta B. At. Spectrosc.* 52, 1955-1963 (1997).

ICP/LIF
As,Sb,Se
Laser Power Dependences
Detection Limits

78060. Xu, L., V. Bulatov, V.V. Gridin and I. Schechter, "Absolute Analysis of Particulate Materials by Laser Induced Breakdown Spectroscopy," *Anal. Chem.* 69, 2103-2108 (1997).

LIBS
Aerosols
Zn
Analysis Method
Detection Limits

78061. Green, R.B., and M.D. Seltzer, "Laser Induced Ionization Spectrometry," One of Five Reviews, 238 pp., Edited by J. Sneddon, in *Advances in Atomic Spectroscopy* 1, 37-79 (1992).

Atomic Analysis
Laser Induced Ionization Methods
Detection Limits
Review

78062. Gibson, J.K., "Resonant Laser Ablation of Lanthanides: Eu and Lu Resonances in the 450-470 nm Region," *Anal. Chem.* 69, 111-117 (1997).

Laser Ablation
Mass Analysis
Lanthanides
M^+,MO^+ Plumes

78063. Gittins, C.M., M.J. Castaldi, S.M. Senkan and E.A. Rohlfing, "Real-Time Quantitative Analysis of Combustion Generated Polycyclic Aromatic Hydrocarbons by Resonance-Enhanced Multiphoton Ionization Time-of-Flight Mass Spectrometry," *Anal. Chem.* 69, 286-293 (1997).

Mass Analysis/ REMPI
$C_{10}H_8$,$C_{13}H_{10}$
$C_{14}H_{10}$ PAHS
Monitor
$CH_4/O_2/Ar$
Diffusion Flame

78064. Pupyshev, A.A., A.N. Gubanova and K.F. Byl'chenko, "Study of the Analytical Possibilities of Acetylene/Nitric Oxide and Propane (Butane)/Nitric Oxide Flames," *J. Anal. Chem., Russia* 50, 158-160 (1995).

Atomic Analysis
Absorption
C_2H_2/NO
C_3H_8,C_4H_{10}/NO
Flames
Detection Limits

(78073) 431 nm Laser Absorption, $CH_4/O_2/Ar$ and CH_4/O_2 NO/Ar Mixtures, Shock Tube, Profiles, Comparisons

CH

78065. Goehlich, A., T. Kawetzki and H.F. Dobele, "On Absolute Calibration with Xenon of Laser Diagnostic Methods Based on Two-Photon Absorption," *J. Chem. Phys.* 108, 9362-9370 (1998).

2-Photon Absorption
O-Atom
Species Densities
Xe Calibration Method

78066.	Paul, J.B., and R.J. Saykally, "Cavity Ringdown Laser Absorption Spectroscopy," *Anal. Chem.* 69(9), 287A-292A (1997).	Laser Absorption Cavity Ringdown Analysis Method Overview
(78024)	633 nm He-Ne Laser, Isotopic Monitoring Method, CO_2, N_2, O_2, Air Quenching Effects	LIF,I_2(B-X)
(77834)	N,O/Quartz, Heterogeneous Recombination Coefficients, Atom Monitoring	2-Photon LIF
78067.	Ravikrishna, R.V., and N.M. Laurendeau, "Laser Saturated Fluorescence Measurements of Nitric Oxide in Laminar Counterflow Diffusion Flames," *Combust. Flame* 113, 473-475 (1998).	Saturated LIF NO Counterflow Diffusion Flame Measurements
(77657)	Gasoline Octane Number, Spectral Monitoring Method	Raman
78068.	Boyarshinov, B.F., S.Yu. Fyodorov and A.A. Volkov, "CARS Measurements of the Correlation of Scalar Parameters in a Hydrogen Jet and Flame," *Heat Transfer Res.* 27, 169-173 (1996).	CARS T,H_2 Densities Turbulent H_2 Jet
78069.	Schmitt, M., G. Knopp, A. Materny and W. Kiefer, "The Application of Femtosecond Time-Resolved Coherent Anti-Stokes Raman Scattering for the Investigation of Ground and Excited State Molecular Dynamics of Molecules in the Gas Phase," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4059-4065 (1998).	fs CARS Br_2,I_2(A,X) Reaction Dynamics Monitor
78070.	Wasserman, T.A.W., P.H. Vaccaro and B.R. Johnson, "Degenerate Four-Wave Mixing Spectroscopy as a Probe of Orientation and Alignment in Molecular Systems," *J. Chem. Phys.* 108, 7713-7738 (1998).	DFWM Rotational Anisotropy Monitor
78071.	Fernee, M.J., P.F. Barker, A.E.W. Knight and H. Rubinsztein-Dunlop," *Phys. Rev. Lett.* 79, 2046-2049 (1997).	2-Photon 4-Wave Mixing NO(C-X) Enhanced Sensitivity Monitoring Method
78072.	Fernee, M.J., P.F. Barker, A.E.W. Knight and H. Rubinsztein-Dunlop, "Sensitive Detection of Nitric Oxide Using Seeded Parametric Four-Wave Mixing," *J. Chem. Phys.* 108, 6291-6302 (1998).	4-Wave Mixing NO(C-X) Sensitive Monitoring Method C_2H_2/Air Flame
(78129)	NaH + NaH Rate Constant, NaH/H_2 Diffusion Constant	DFWM,NaH

31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

78073.	Woiki, D., M. Votsmeier, D.F. Davidson, R.K. Hanson and C.T. Bowman, "CH Radical Concentration Measurements in Fuel-Rich $CH_4/O_2/Ar$ and $CH_4/O_2/NO/Ar$ Mixtures Behind Shock Waves," *Combust. Flame* 113, 624-626 (1998).	CH Species Profiles $CH_4/O_2/Ar$ $CH_4/O_2/NO/Ar$ Comparisons Shock Tube Laser Absorption
78074.	Bhargava, A., and P.R. Westmoreland, "Measured Flame Structure and Kinetics in a Fuel-Rich Ethylene Flame," *Combust. Flame* 113, 333-347 (1998).	Species Profiles C_2H_4/O_2 Molecular Beam Mass Analysis Fuel Rich C_2H_4+OH,H C_2H_3/C_2H_2+H Rate Constants
(78067)	Counterflow Diffusion Flame Measurements, Satured LIF	NO
78075.	Korobeinichev, O.P., V.M. Shvartsberg and S.B. Il'in, "Destruction Chemistry of Organophosphorus Compounds in Hydrogen/Oxygen Flames," *Combust. Expl. Shock Waves, Russia* 33, 270-283 (1997).	Species Profiles $H_2/O_2/Ar$ $CH_3PO(OCH_3)_2$ $(CH_3)_3PO_4$ Products Mass Spectra

32. MAPPING/TOMOGRAPHIC METHODS

78076.	Heck, A.J.R., and D.W. Chandler, "Imaging Techniques for the Study of Chemical Reaction Dynamics," *Ann. Rev. Phys. Chem.* 46, 335-372 (1995).	Imaging $CH_3I,CD_3I+h\nu$ $C_2H_2,HI,DI,O_3+h\nu$ $H+HI,D_2$ $NO(^2\Pi)+Ar$ Products,Methods Review
(78166)	Product Velocity Ion Imaging, $CH_3Br+h\nu$, Br/Br* Branching, A-State Lifetime	Br,CH_3
(78189)	Sub ps Probe, $CH_3COCl+h\nu$, Unimolecular Dissociation	CH_3CO Imaging
(77769)	OH, LIF, Rayleigh Temperatures, Turbulent CH_4, CH_3OH, C_2H_5OH Diffusion Flames	Imaging
78077.	Baum, R.T., K.B. McGrattan and M.R. Nyden, "An Examination of the Applicability of Computed Tomography for the Measurement of Component Concentrations in Fire Generated Plumes," *Combust. Flame* 113, 358-372 (1998).	Tomography Fire Plumes Feasibility Assessments

(77904) Particle Sizes, Densities, 2-Phase Turbulent Coaxial Jet, Laser Diffraction Method — Tomography

33. OPTOGALVANIC/OPTOACOUSTIC METHODS

78078. Rai, S.B., and D.K. Rai, "Optogalvanic Spectroscopy," *Proc. Indian Natl. Sci. Acad. A* (New Delhi) 62, 475-512 (1996).

Optogalvanic Spectroscopy
Atoms,Molecules
Tabulated Studies
Review

(77666) Optoacoustic Monitoring, Coal, Peat, Woodchip FBC — NO,SO_2

34. FLAME KINETIC MODELING

78079. Law, C.K., "The Role of Chain Mechanisms in Some Fundamental Combustion Phenomena," pp. 3-27 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).

Combustion Kinetics
Chain Mechanism
Modeling Needs
Review

78080. Eiteneer, B., C.-L. Yu, M. Goldenberg and M. Frenklach, "Determination of Rate Coefficients for Reactions of Formaldehyde Pyrolysis and Oxidation in the Gas Phase," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5196-5205 (1998).

Kinetic Modeling
CH_2O/Ar
CH_2O/O_2/Ar
CO Product Rates
Shock Tube
Sensitivity Analysis

78081. Dautov, N.G., and A.M. Starik, "On the Problem of Choosing a Kinetic Scheme for the Homogeneous Reaction of Methane with Air," *Kinet. Catal., Russia* 38, 185-208 (1997).

Kinetic Modeling
CH_4/Air
CH_4/O_2/Ar
433 Reactions
Reduced Scheme
Adequacies

78082. Seshadri, K., X.S. Bai, H. Pitsch and N. Peters, "Asymptotic Analysis of the Structure of Moderately Rich Methane/Air Flames," *Combust. Flame* 113, 589-602 (1998).

Reduced Kinetics
CH_4/Air
Flame Structure
Rich Premixed
Asymptotic Analysis
Burning Velocities

78083. Chou, C.-P., J.-Y. Chen, C.G. Yam and K.D. Marx, "Numerical Modeling of NO Formation in Laminar Bunsen Flames: A Flamelet Approach," *Combust. Flame* 114, 420-435 (1998).

Kinetic Modeling
Rich CH_4
Bunsen Flame
Flamelet Concept
CO,NO Formation

78084. Park, Y.K., and D.G. Vlachos, "Isothermal Chain-Branching, Reaction Exothermicity, and Transport Interactions in the Stability of Methane/Air Mixtures," *Combust. Flame* 114, 214-230 (1998).

Kinetic Modeling
CH_4/Air
Stirred Reactor
Exothermically Driven Instabilities
Sensitivity Analysis

(77814) Kinetic Modeling, Flame Speeds, Inhibition Effects

CH_4/Air/$CHCl_3$
CH_4/Air/CH_2Cl_2

78085. Eggels, R.L.G.M., J.J.J. Louis, J.B.W. Kok and L.P.H. De Goey, "Comparison of Conventional and Low-Dimensional Manifold Methods to Reduce Reaction Mechanisms," *Combust. Sci. Technol.* 123, 347-362 (1997).

Kinetic Modeling
$CO/H_2/O_2$
H_2/O_2
Reduced Schemes
Comparisons

78086. Mueller, C., P. Kilpinen and M. Hupa, "Influence of HCl on the Homogeneous Reactions of CO and NO in Postcombustion Conditions: A Kinetic Modeling Study," *Combust. Flame* 113, 579-588 (1998).

Kinetic Modeling
CO Oxidation
CO,NO
Burnt Gases
HCl Effects

78087. Kuzovnikov, A.A., A.V. Ponomareva and V.S. Sviridkina, "Increased Degree of Conversion of CO to CO_2 Due to Water Dissociation in Plasmochemical Systems," *Moscow Univ. Phys. Bull.* 50(3), 17-22 (1995).

Kinetic Modeling
$CO/O_2/H_2O$
Enhanced CO_2 Formation
Plasma Assistance

78088. Lindstedt, R.P., and G. Skevis, "Chemistry of Acetylene Flames," *Combust. Sci. Technol.* 125, 73-137 (1997).

Kinetic Modeling
$C_2H_2/O_2/N_2$
Lean/Rich Flames
Data Comparisons

78089. Peeters, J., "Key Reactions in the Oxidation of Acetylene by Atomic Oxygen," *Bull. Soc. Chim. Belg.* 106, 337-342 (1997).

Kinetic Modeling
C_2H_2/O_2
Key Reactions
$CHCO, C_2H, C_3H_2$
$CH(A,X), CH_2(a,X)$
Rate Constants
Mechanisms
Review

78090. Dagaut, P., N. Smoucovit and M. Cathonnet, "Methyl Acetate Oxidation in a Jet Stirred Reactor: Experimental and Detailed Kinetic Modeling Study," *Combust. Sci. Technol.* 127, 275-291 (1997).

Kinetic Modeling
CH_3COOCH_3/O_2
Species Profiles
Probe/GC Analysis
Sensitivity Analysis

(77707) Primary Flame Kinetic Modeling, $(CH_2NNO_2)_3$, Deflagration Velocities

RDX

78091. Warth, V., N. Stef, P.A. Glaude, F. Battin-Leclerc, G. Scacchi and G.M. Come, "Computer-Aided Derivation of Gas Phase Oxidation Mechanisms: Application to the Modeling of the Oxidation of *n*-Butane," *Combust. Flame* 114, 81-102 (1998).

Kinetic Modeling
n-C_4H_{10}/O_2
Computer Aided Mechanism Formulation
Large Reaction Schemes

78092. Marinov, N.M., W.J. Pitz, C.K. Westbrook, A.M. Vincitore, M.J. Castaldi, S.M. Senkan and C.F. Melius, "Aromatic and Polycyclic Aromatic Hydrocarbon Formation in a Laminar Premixed *n*-Butane Flame," *Combust. Flame* 114, 192-213 (1998).

Kinetic Modeling
n-$C_4H_{10}/O_2/Ar$
PAH,Aromatics
Species Profiles
Data Comparisons

78093. Curran, H.J., P. Gaffuri, W.J. Pitz and C.K. Westbrook, "A Comprehensive Modeling Study of *n*-Heptane Oxidation," *Combust. Flame* 114, 149-177 (1998).

Kinetic Modeling
n-C_7H_{16}/O_2
Ignition Delays
Data Comparisons
Sensitivity Analysis

78094. Zhao, J., K.M. Isaac and G.L. Pellett, "Global Characteristics and Structure of Hydrogen/Air Counterflow Diffusion Flames," Presented Originally as AIAA Paper 94-0680 at the *32nd AIAA Aerospace Sciences Meeting and Exhibit*, Held in Reno NV, January 1994, *J. Propulsion Power* 12, 534-542 (1996).

Kinetic Modeling
H_2/Air
Counterflow
Species Profiles
Characterization

78095. Sanchez, A.L., A. Linan and F.A. Williams, "A Generalized Burke-Schumann Formulation for Hydrogen/Oxygen Diffusion Flames Maintaining Partial Equilibrium of the Shuffle Reactions," *Combust. Sci. Technol.* 123, 317-345 (1997).

Kinetic Modeling
H_2/O_2
Diffusion Flames
Partial Equilibrium
Reduced Scheme

(77816) Kinetic Modeling, Species Profiles, Inhibition Effects

$H_2/Air/C_3HF_7$

35. PYROLYSIS KINETICS/STUDIES

78096. Miller, R.S., and J. Bellan, "Tar Yield and Collection from the Pyrolysis of Large Biomass Particles," *Combust. Sci. Technol.* 127, 97-118 (1997).

Pyrolysis
Biomass Particles
Tar Yields

(78080) Shock Tube Pyrolysis/Oxidation, CO Product Rates, Kinetic Modeling, Sensitivity Analysis

CH_2O/Ar
$CH_2O/O_2/Ar$

78097. Zaslonko, I.S., Yu.P. Petrov and V.N. Smirnov, "Thermal Decomposition of Nitromethane in Shock Waves: The Effect of Pressure and Collision Partners," *Kinet. Catal., Russia* 38, 321-324 (1997).

Pyrolysis
CH_3NO_2+M
Rate Constants
Fall-off Parameters
M = He,Ar,CF_4,CO_2
Shock Tube

(77704) Pyrolysis, Energetic Materials, Product Infrared, Mass Analysis

c-$RR'C_2N_2O$

78098. Esker, D.R., and M.Q. Brewster, "Laser Pyrolysis of Hydroxyl Terminated Polybutadiene," *J. Propulsion Power* 12, 296-301 (1996).

IR Laser Pyrolysis
Polybutadiene
Regression Rate
Surface Temperature
Activation Energy

78099. Held, T.J., A.J. Marchese and F.L. Dryer, "A Semi-Empirical Reaction Mechanism for *n*-Heptane Oxidation and Pyrolysis," *Combust. Sci. Technol.* 123, 107-146 (1997).

Pyrolysis/
Oxidation
n-C_7H_{16}
Reaction
Mechanism

78100. Zaslonko, I.S., and Yu.K. Mukoseev, "Thermal Decomposition of $SiCl_4$ in Shock Waves," *Kinet. Catal., Russia* 38, 325-329 (1997).

Pyrolysis
$SiCl_4 + Ar$
Rate Constants
T Dependence
Shock Tube

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 35 for Pyrolysis Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

78101. Tomlin, A.S., T. Turanyi and M.J. Pilling, "Mathematical Tools for the Construction, Investigation and Reduction of Combustion Mechanisms," Chapter 4 in *Low Temperature Combustion and Autoignition*, M.J. Pilling, ed., 7 Chapters, 794 pp., *Comprehensive Chemical Kinetics* 35, 293-437 (1997).

Kinetic Modeling
Scheme Reduction
Techniques
Review

78102. Golden, D.M., and J.A. Manion, "Applications of Chemical Kinetics," in *Advances in Chemical Kinetic and Dynamics*, J.R. Barker, ed., 5 Reviews, 280 pp., Volume 1, 187-276 (1992).

Rate Constants
Thermochemistry
Applications
SRI Program
Review

78103. Sims, I.R., and I.W.M. Smith, "Gas Phase Reactions and Energy Transfer at Very Low Temperatures," *Ann. Rev. Phys. Chem.* 46, 109-137 (1995).

Rate Constants
$CN + C_2H_2, C_2H_6, O_2$
$CO_2(v) + CO$
$OH + HBr$
Low Temperatures
Review

78104. Michael, J.V., "The Measurement of Thermal Bimolecular Rate Constants by the Flash Photolysis-Shock Tube Technique: Comparison of Experiment to Theory," in *Advances in Chemical Kinetic and Dynamics*, J.R. Barker, ed., 5 Reviews, 280 pp., Volume 1, 47-112 (1992).

Rate Constants
$H + H_2O, D_2O, O_2$
$D + H_2, H + NH_3$
$O + CH_4, C_2H_2, C_2D_2$
$O + H_2, D_2, H_2O$
Photolysis/Shock Tube
Isotope Effects
Measurements

(77999) Rate Constants, $^2P_{1/2,3/2}$ Spin-Orbit Effects, Temperature Dependences, Calculations — $Al+O_2$

78105. Berry, R.J., J. Yuan, A. Misra and P. Marshall, "Experimental and Computational Investigations of the Reaction of OH with CF_3I and the Enthalpy of Formation of HOI," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5182-5188 (1998).
CF_3I+OH
Rate Constants
Channels
$\Delta H_f(HOI)$

78106. Robertson, S.H., P.W. Seakins and M.J. Pilling, "Elementary Reactions," Chapter 2 in *Low Temperature Combustion and Autoignition*, M.J. Pilling, ed., 7 Chapters, 794 pp., *Comprehensive Chemical Kinetics* 35, 125-234 (1997).
Hydrogen
Oxidation
Radicals
Rate Constant
Measurements
Review

78107. Baulch, D.L., "Kinetics Databases," Chapter 3 in *Low Temperature Combustion and Autoignition*, M.J. Pilling, ed., 7 Chapters, 794 pp., *Comprehensive Chemical Kinetics* 35, 235-292 (1997).
Hydrocarbon
Oxidation
Rate Constants
Kinetic Database
Assessments
Review

78108. Atkinson, R., "Gas Phase Tropospheric Chemistry of Organic Compounds," *J. Phys. Chem. Ref. Data Monograph* No. 2, 216 pp. (1994).
Organics$+NO_3$,OH
Organics$+O_3$
Rate Constants
Mechanisms
Monograph

78109. Denisov, E.T., and V.E. Tumanov, "The Force Constant of the C-X Bond as a Factor Determining the Activation Energy of the X-Atom Radical Abstraction Reactions (X=Cl, Br and I)," *Kinet. Catal., Russia* 38, 345-349 (1997).
Activation Energies
$R'+RX$
$H+RX$
R=Alkyl
X=Cl,Br,I
RX Force Constant
Correlation

78110. Benson, S.W., and O. Dobis, "Existence of Negative Activation Energies in Simple Bimolecular Metathesis Reactions and Some Observations on Too-Fast Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5175-5181 (1998).
Negative
Activation Energies
$R+HX$
$R+X_2$
R=Alkyl
Experimental
Artifact

78111. Fulle, D., H. Hippler and F. Striebel, "The High Pressure Range of the Reaction $CH(^2\Pi)+CO+M\rightarrow HCCO+M$," *J. Chem. Phys.* 108, 6709-6716 (1998).
$CH+CO+M$
Rate Constants
Fall-off Parameters
T Dependence

78112. Rim, K.T., and J.F. Hershberger, "A Diode Laser Study of the Product Branching Ratios of the $CH+NO_2$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4592-4595 (1998).
$CH+NO_2$
Branching Ratios
Product Yields

78113. Tyndall, G.S., T.J. Wallington and J.C. Ball, "FTIR Product Study of the Reactions $CH_3O_2+CH_3O_2$ and $CH_3O_2+O_3$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2547-2554 (1998).

$CH_3O_2+O_3$
$(CH_3)_2N_2+Cl$
Rate Constants
$CH_3O_2+CH_3O_2$
Branching Ratio
Products

78114. Edwards, M.A., and J.F. Hershberger, "Kinetics of the $CN+CH_2CO$ and $NCO+CH_2CO$ Reactions," *Chem. Phys.* 234, 231-237 (1998).

$CN+CH_2CO$
$NCO+CH_2CO$
Rate Constants
T Dependences
CO Product Yields

78115. He, G., I. Tokue and R.G. Macdonald, "Thermal Rate Constant for $CN+H_2/D_2 \rightarrow HCN/DCN+H/D$ Reaction from 293 to 380 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4585-4591 (1998).

$CN+H_2$
$CN+D_2$
Rate Constants
T Dependences

(78089) Kinetic Modeling, CHCO, C_2H, C_3H_2, CH(A,X), CH_2(a,X) Key Reactions, Rate Constants, Mechanisms, Review

C_2H_2/O_2

(78074) Rate Constants, Fuel Rich C_2H_4/O_2 Flame, Molecular Beam/Mass Analysis Species Profiles

C_2H_4+H,OH
C_2H_2,C_2H_3+H

78116. Platz, J., L.K. Christensen, J. Sehested, O.J. Nielsen, T.J. Wallington, C. Sauer, I. Barnes, K.H. Becker and R. Vogt, "Atmospheric Chemistry of 1,3,5-Trioxane: Ultraviolet Spectra of *c*-$C_3H_5O_3$ and (*c*-$C_3H_5O_3$)O_2 Radicals, Kinetics of the Reactions of (*c*-$C_3H_5O_3$)O_2 Radicals with NO and NO_2, and Atmospheric Fate of the Alkoxy Radical (*c*-$C_3H_5O_3$)O," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4829-4838 (1998).

2 *c*-$C_3H_5O_3$
c-$C_3H_5O_3+O_2$
(*c*-$C_3H_5O_3$)O_2+NO
(*c*-$C_3H_5O_3$)O_2+NO_2
c-$C_3H_6O_3$+F,Cl,OH
HC(O)OCH_2OC(O)H+Cl
Rate Constants
c-$C_3H_5O_3$,(*c*-$C_3H_5O_3$)O_2
UV Spectrum
(*c*-$C_3H_5O_3$)O_2NO_2
IR Spectrum

78117. Zhong, X., and J.W. Bozzelli, "Thermochemical and Kinetic Analysis of the H, OH, HO_2, O and O_2 Association Reactions, with Cyclopentadienyl Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3537-3555 (1998).

c-C_5H_5+H,O,OH
c-$C_5H_5+HO_2,O_2$
Thermochemical
Estimated Energies
Channels
High Pressure
Rate Constants

78118. Christensen, L.K., J. Sehested, O.J. Nielsen, M. Bilde, T.J. Wallington, A. Guschin, L.T. Molina and M.J. Molina, "Atmospheric Chemistry of HFE-7200 ($C_4F_9OC_2H_5$): Reaction with OH Radicals and Fate of $C_4F_9OCH_2CH_2O$ and $C_4F_9OCH(O)CH_3$ Radicals," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4839-4845 (1998).

n-$C_4F_9OC_2H_5$+OH
i-$C_4F_9OC_2H_5$+OH
$C_4F_9OC_2H_5$+F,Cl
$C_4F_9OC(O)CH_3$+Cl
Rate Constants
Atmospheric
Lifetimes

78119. Kramp, F., and S.E. Paulson, "On the Uncertainties in the Rate Coefficients for OH Reactions with Hydrocarbons, and the Rate Coefficients of the 1,3,5-Trimethylbenzene and *m*-Xylene Reactions with OH Radicals in the Gas Phase," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2685-2690 (1998).

$C_6H_4(CH_3)_2 + OH, O_3$
$C_6H_3(CH_3)_3 + OH, O_3$
$(C_4H_9)_2O + OH$
c-$C_6H_{11}CH_3 + OH$
c-C_5H_{10}, *c*-$C_6H_{12} + OH$
$C_6H_5CH_3 + OH$
Rate Constants

78120. Sommer, T., and P. Roth, "High Temperature Reactions of Fullerene C_{60} with H and OH," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3083-3088 (1998).

$C_{60} + H$
$C_{60} + OH$
Rate Constants
T Dependences
Shock Tube

78121. Notario, A., G. Le Bras and A. Mellouki, "Absolute Rate Constants for the Reactions of Cl Atoms with a Series of Esters," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3112-3117 (1998).

$Cl + HCOOR$
$Cl + R'COOR$
Rate Constants
$R = C_1$-C_4 Alkyl
$R' = C_1$-C_5Alkyl
Measurements

78122. Farrell, J.T., and C.A. Taatjes, "Infrared Frequency-Modulation Probing of $Cl + C_3H_4$ (Allene, Propyne) Reactions: Kinetics of HCl Production from 292 to 850 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4846-4856 (1998).

$Cl + CH_2CCH_2$
$Cl + CH_3CCH$
Rate Constants
HCl Product
T,P Dependences

78123. Baer, M., M. Faubel, B. Martinez-Haya, L.Y. Rusin, U. Tappe and J.P. Toennies, "State-to-State Differential Cross Sections for the Reaction $F + D_2$ at 90 meV: A Crossed Molecular Beam Experiment and a Quantum Mechanical Study," *J. Chem. Phys.* 108, 9694-9710 (1998).

$F + D_2$
2.07 kcal mol^{-1}
Collision Energy
DF(v,J) Product
Cross Sections
Crossed Beam
Experiments

78124. Banares, L., F.J. Aoiz, V.J. Herrero, M.J. D'Mello, B. Niederjohann, K. Seekamp-Rahn, E. Wrede and L. Schnieder, "Experimental and Quantum Mechanical Study of the $H + D_2$ Reaction Near 0.5 eV: The Assessment of the H_3 Potential Energy Surfaces," *J. Chem. Phys.* 108, 6160-6169 (1998).

$H + D_2$
Reactive
Cross Sections
Measurements
P.E. Surface
Calculation
Accuracies

78125. Hawthorne, G., P. Sharkey and I.W.M. Smith, "Rate Coefficients for the Reaction and Relaxation of Vibrationally Excited $H_2O(|04\rangle^-)$ with H Atoms and H_2O," *J. Chem. Phys.* 108, 4693-4696 (1998).

$H_2O(4\nu_{OH}) + H$
$H_2O(4\nu_{OH}) + H_2O$
Rate Constants
Relaxation
Reaction Channels

78126.	Loesch, H.J., "Orientation and Alignment in Reactive Beam Collisions: Recent Progress," *Ann. Rev. Phys. Chem.* 46, 555-594 (1995).	K+ICl Li+HF Cross Sections Steric/Alignment Effects Review
78127.	Deschamps, J., and J.L. Godart, "Temperature Dependence of the Rate of the Reaction N+H+Ar→NH+Ar," *Contrib. Plasma Phys.* 35, 127-131 (1995).	N+H+Ar Rate Constants 550-750 K $Ar/N_2/H_2$ Discharge
78128.	Mebel, A.M., and M.C. Lin, "Reactions of NO_x with Nitrogen Hydrides," *Int. Rev. Phys. Chem.* 16, 249-266 (1997).	$NO+NH,NH_2,NH_3$ NO_2+NH,NH_2,NH_3 Rate Constants Branching Ratios Measurements Calculations Review
78129.	Lehr, L., M. Motzkus, G. Pichler and P. Hering, "Determination of the Reaction Dynamics of Sodium Hydride in a Hydrogen Atmosphere with Degenerate Four-Wave Mixing," *J. Raman Spectrosc.* 29, 273-282 (1998).	NaH+NaH Rate Constant NaH/H_2 Diffusion Constant DFWM Monitor
78130.	Donahue, N.M., J.G. Anderson and K.L. Demerjian, "New Rate Constants for Ten OH Alkane Reactions from 300 to 400 K: An Assessment of Accuracy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3121-3126 (1998).	OH+Alkanes Rate Constants T Dependences Measurements Data Comparisons 10 Alkanes
78131.	Le Calve, S., D. Hitier, G. Le Bras and A. Mellouki, "Kinetic Studies of OH Reactions with a Series of Ketones," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4579-4584 (1998).	OH+Ketones Rate Constants 5 Molecules T Dependences Measurements
78132.	Fulle, D., H.F. Hamann, H. Hippler and J. Troe, "Temperature and Pressure Dependence of the Addition Reactions of HO to NO and to NO_2. IV. Saturated Laser Induced Fluorescence Measurements up to 1400 bar," *J. Chem. Phys.* 108, 5391-5397 (1998).	OH+NO+M $OH+NO_2+M$ Rate Constants Fall-off Parameters 250-400 K Measurements
78133.	Toby, S., and F.S. Toby, "Reactivity of the Ozone/Ethane System," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4527-4531 (1998).	$O_3+C_2H_6$ 24-150 °C Reactivity Induction Periods O_2 Effects Kinetic Modeling

78134. De Silva, K.M.N., and D. Husain, "Bromine Atom-Abstraction Reactions at Elevated Temperatures by Ground State Atomic Rubidium, Rb($5^2S_{1/2}$), Investigated by Time-Resolved Laser Induced Fluorescence (Rb($5^2P_{3/2}$-$5^2S_{1/2}$) 780 nm)," *J. Photochem. Photobiol. A. Chem.* 111, 1-7 (1997).

Rb+RBr
Rate Constants
R=C_1-C_6 Alkyl

78135. Carl, S.A., K.M.N. De Silva and D. Husain, "Kinetic Investigation of Chlorine Atom-Abstraction Reactions by Ground State Atomic Rubidium, Rb($5^2S_{1/2}$), by Time-Resolved Laser Induced Fluorescence [Rb($5^2P_{3/2}$-$5^2S_{1/2}$) 780 nm] Following Pulsed Irradiation," *Z. Phys. Chem. (Munchen)* 203, 113-130 (1998).

Rb+RCl
Rate Constants
R=C_1-C_7 Alkyl

78136. Shiina, H., A. Miyoshi and H. Matsui, "Investigation on the Insertion Channel in the S(^{3}P)+H_2 Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3556-3559 (1998).

S+H_2+M
Rate Constant
Spin Forbidden
H_2S Product
Channel

78137. Kochubei, V.F., "Kinetics of the Gas Phase Hydrolysis of Silicon Tetrachloride," *Kinet. Catal., Russia* 38, 212-214 (1997).

$SiCl_4$+H_2O
Rate Constant
T Dependence
293-373 K
740-970 K

(77818) Low Pressure Glow Discharges, Deposition Reaction Scheme, Rate Constants Review

SiH_4

78138. Campbell, M.L., "Temperature Dependent Study of the Gas Phase Kinetics of Zr(a^3F_2) and Hf(a^3F_2)," *J. Chem. Soc., Faraday Trans.* 94, 1687-1693 (1998).

Zr+M
Hf+M
Rate Constants
M=7 Species
T Dependences
P Independences

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

78139. Valentini, J.J., "State-to-State Dynamics: Do We Really Need All Those Data?," in *Advances in Chemical Kinetic and Dynamics*, J.R. Barker, ed., 5 Reviews, 280 pp., Volume 1, 1-45 (1992).

Photofragmentation
State-to-State
Dynamics
H+HX
O_3+hν
Review

78140. Baklashova, V.E., B.F. Gordiets and A.I. Osipov, "Thermal Explosion During Laser Dissociation of Molecular Gas," *Moscow Univ. Phys. Bull.* 48(6), 50-55 (1993).

MPD
Diatomics
Recombination
Heating
Thermal Explosion
Modeling

(77908)	Photochemistry, van der Waals Complexes, Small Clusters, Review	Clusters+hν
(77793)	Photoionization/Dissociation, Product Ions, Channels	CCl_2F_2+hν
78141.	del Barrio, J.I., R.F. Cezar and F.M. G-Tablas, "Effect of NO on the Isotopically Selective Dissociation of CF_3Br with a Transversely Excited Atmospheric CO_2 Laser," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3215-3218 (1998).	CF_3Br+hν IR Dissociation Isotopic Enrichment NO Enhancement Effects
78142.	Marvet, U., Q. Zhang and M. Dantus, "Femtosecond Dynamics of Unimolecular and Unrestricted Bimolecular Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4111-4117 (1998).	CH_2I_2+hν I_2 Product Hg+Hg+hν Photoassociation fs Pump/Probe Monitoring
(78076)	Product Imaging Techniques, Review	CH_3I,CD_3I+hν C_2H_2,HI,DI,O_3+hν
(78183)	Unimolecular Photodissociation, Review	CH_3O,HCO HFCO,NO_2
(77909)	Comparisons of Half-Collision Reactions with H+CO_2 and Br+I_2 Dynamics, Review	CO_2.HX+hν HBr.I_2+hν
78143.	Mellinger, A., M.V. Ashikhmin and C.B. Moore, "Experimental Evidence for K-Conservation in the Dissociation of Singlet Ketene," *J. Chem. Phys.* 108, 8944-8949 (1998).	CH_2CO+hν Dynamics Product CH_2 LIF Monitor K Mixing/ Conservation
78144.	Blank, D.A., W. Sun, A.G. Suits, Y.T. Lee, S.W. North and G.E. Hall, "Primary and Secondary Processes in the 193 nm Photodissociation of Vinyl Chloride," *J. Chem. Phys.* 108, 5414-5425 (1998).	C_2H_3Cl+hν Product Photofragments Primary/ Secondary Channels
(78189)	Unimolecular Dissociation, CH_3CO Fragment, Sub ps Probe, Ion Imaging	CH_3COCl+hν
78145.	Gordienko, V.M., E.O. Danilov, N.Yu. Ignatieva, V.V. Timofeev and Yu.N. Zhitnev, "Multiphoton Dissociation of Ethylene Under the Action of 10 μm Radiation of a Picosecond Laser: Generation of Vinylidene," *Bull. Russian Acad. Sci., Phys.* 60, 401-407 (1996).	C_2H_4 IR MPD ps/ns Pulses CCH_2 Formation
(77798)	1-Photon Ionization, $C_2H_5SH^+$+Ar Collisional Dissociation, Product Ions, Comparisons	C_2H_5SH+hν

78146.	Winter, P.R., B. Rowland, W.P. Hess, J.G. Radziszewski, M.R. Nimlos and G.B. Ellison, "Ultraviolet Photodissociation of Matrix Isolated Propionyl Chloride," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3238-3248 (1998).	$C_2H_5COCl + h\nu$ FTIR Product Analysis C_2H_5COCl, CH_2CO CH_3CHCO Frequencies Matrix Study
78147.	Scala, A.A., E.W.-G. Diau, Z.H. Kim and A.H. Zewail, "Femtosecond β-Cleavage Dynamics: Observation of the Diradical Intermediate in the Nonconcerted Reactions of Cyclic Ethers," *J. Chem. Phys.* 108, 7933-7936 (1998).	$c\text{-}C_4H_4O$ fs MPD Product Mass Analysis Channels
(78184)	Unimolecular Bond Fission, RRKM Theory, Review	$t\text{-}C_4H_9NO + h\nu$ $NCNO + h\nu$
78148.	DeWitt, M.J., and R.J. Levis, "The Role of Electron Delocalization in the Ionization of C_6 Hydrocarbons Using Intense 780 nm Laser Pulses of Femtosecond Duration," *J. Chem. Phys.* 108, 7045-7048 (1998).	C_6H_6, C_6H_8 C_6H_{12}, C_6H_{14} MPD/MPI fs Laser Pulses Ion Yields
(77911)	355 nm Induced Thermionic Emission, Delayed Electron Efficiency	$C_{60} + h\nu$
78149.	Ekern, S.P., A.G. Marshall, J. Szczepanski and M. Vala, "Photodissociation of Gas Phase Polycyclic Aromatic Hydrocarbon Cations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3498-3504 (1998).	$C_{60}^+ + h\nu$ $PAH^+ + h\nu$ UV/Visible Fragmentation Patterns 24 PAHS
78150.	Lin, J.J., D.W. Hwang, Y.T. Lee and X. Yang, "Photodissociation Dynamics of OClO at 157 nm," *J. Chem. Phys.* 108, 10061-10069 (1998).	$ClO_2 + h\nu$ Channels Branching Ratios ClO(v) Product Dynamics
78151.	Trushin, S.A., W. Fuss, W.E. Schmid and K.L. Kompa, "Femtosecond Dynamics and Vibrational Coherence in Gas Phase Ultraviolet Photodecomposition of $Cr(CO)_6$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4129-4137 (1998).	$Cr(CO)_6 + h\nu$ Photochemical Mechanism fs Pump/Probe
78152.	Gutmann, M., J.M. Janello, M.S. Dickebohm, M. Grossekathofer and J. Lindener-Roenneke, "Ultrafast Dynamics of Transition Metal Carbonyls: Photodissociation of $Cr(CO)_6$ and $Cr(CO)_6.(CH_3OH)_n$ Heteroclusters at 280 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4138-4147 (1998).	$Cr(CO)_6 + h\nu$ $Cr(CO)_6.(CH_3OH)_n + h\nu$ Product MPI Fragmentation Patterns

78153. Garcia-Vela, A., "Study of the Total and Partial Fragmentation Dynamics of Ar-HCl after Ultraviolet Photodissociation," *J. Chem. Phys.* 108, 5755-5766 (1998).

$HCl.Ar + h\nu$
Photodissociation
Dynamics
Channels
Products

(77958) OH Product Quantum Yields, Ultraviolet-Visible Absorption Cross Sections

$HOI + h\nu$

78154. Manz, J., M. Oppel and G.K. Paramonov, "Quasi-Coherent Molecular Vibrations with Energies above the Dissociation Threshold in the Ground Electronic State," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4271-4276 (1998).

$HONO_2$
fs IR MPA
Above Dissociation Limit Levels
IR/UV Pump/Probe Monitoring

78155. Tossell, J.A., "Theoretical Study of the Photodecomposition of Methyl Hg Complexes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3587-3591 (1998).

$CH_3HgR + h\nu$
$CH_3Hg^+ + h\nu$
Absorption
Transitions
$R = Cl, Cl^-, CH_3^-, H_2O, OH, OH^-, SH^-$
Frequencies
Calculations

78156. Crepin, C., N. Legay-Sommaire, J.G. McCaffrey and A. Tramer, "Photodissociation of Dimethylmercury in Argon Matrixes by 193 and 248 nm Laser Irradiation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4014-4020 (1998).

$Hg(CH_3)_2 + h\nu$
Product
IR,UV Spectra
Matrix Study

(78231) Low-lying Surfaces, Reactive/E-V Transfer Channels, Theory/Experiment Comparisons

$Na.FH + h\nu$

78157. Peslherbe, G.H., B.M. Ladanyi and J.T. Hynes, "Trajectory Study of Photodissociation Dynamics in the NaI(H_2O) Cluster System," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4100-4110 (1998).

$NaI(H_2O) + h\nu$
Trajectory Calculations
Cluster Effects

78158. Rougeau, N., and C. Kubach, "Theoretical Study of the Photodetachment of $OHCl^-$," *Chem. Phys. Lett.* 274, 535-542 (1997).

$OHCl^- + h\nu$
Photodetachment Spectrum
Calculations

78159. Liou, H.T., S.F. Chiou and K.L. Huang, "Ozone Yields from Oxygen Irradiated at 193 nm," *Ozone Sci. Eng.* 19, 273-280 (1997).

$O_2 + h\nu$ (193 nm)
O_3 Formation
Mechanism
Yields

78160. Takahashi, K., N. Taniguchi, Y. Matsumi, M. Kawasaki and M.N.R. Ashfold, "Wavelength and Temperature Dependence of the Absolute O(^{1}D) Production Yield from the 305-329 nm Photodissociation of Ozone," *J. Chem. Phys.* 108, 7161-7172 (1998).

$O_3 + h\nu$
O(^{1}D) Quantum Yields
305-329 nm
227-295 K

(78289) P.E. Curves, Low-lying States, Processes | $O_3^- + h\nu$

78161. Makarov, G.N., V.N. Lokhman and E. Ronander, "Multiphoton Infrared Absorption by SF_6 in a Gasdynamic Argon Flow," *Opt. Spectrosc., Russia* 83, 215-220 (1997).

SF_6/Ar
IR MPA
Nozzle Cooled
Absorption
Cross Sections

78162. Katagiri, H., T. Sako, A. Hishikawa, T. Yazaki, K. Onda, K. Yamanouchi and K. Yoshino, "Experimental and Theoretical Exploration of Photodissociation of SO_2 via the C^1B_2 State: Identification of the Dissociation Pathway," *J. Mol. Struct.* 413/414, 589-614 (1997).

$SO_2 + h\nu$
Photodissociation
Rates
(C-X) LIF
Quantum Yields
Channels

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions and Section 40 for Theoretically Calculated Reaction Product Distributions)

78163. Morgan, C.G., M. Drabbels and A.M. Wodtke, "Advances in the Measurement of Correlation in Photoproduct Motion," *Adv. Photochem.* 23, 279-350 (1997).

Product States
Photolysis
Correlations
Measurement
Methods
Review

78164. Bonnet, L., and J.C. Rayez, "Comment on the Possibility of Excited Recoil Energy Distributions in the Products of Complex-Forming Reactions with No Exit Barrier," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3455-3456 (1998).

Reaction Products
Translational
Large Energies
Barrierless
Triatomic Systems

78165. Zhong, D., and A.H. Zewail, "Femtosecond Real-Time Probing of Reactions. XXIII. Studies of Temporal, Velocity, Angular and State Dynamics from Transition States to Final Products by Femtosecond-Resolved Mass Spectrometry," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4031-4058 (1998).

Velocity,Angular
Distributions
Reaction Mechanisms
Molecular Beam
fs Mass Analysis
Review

78166. Gougousi, T., P.C. Samartzis and T.N. Kitsopoulos, "Photodissociation Study of CH_3Br in the First Continuum," *J. Chem. Phys.* 108, 5742-5746 (1998).

CH_3,Br
Product Velocity
Ion Imaging
$CH_3Br + h\nu$
Br/Br* Branching
A-State Lifetime

78167.	Moriyama, M., Y. Tsutsui and K. Honma, "Vacuum Ultraviolet Photodissociation Dynamics of Acetonitrile," *J. Chem. Phys.* 108, 6215-6221 (1998).	CN(B),H,D Product Energies $CH_3CN+h\nu$ $CD_3CN+h\nu$ 121.6 nm Mechanism
78168.	Blank, D.A., A.G. Suits, Y.T. Lee, S.W. North and G.E. Hall, "Photodissociation of Acrylonitrile at 193 nm: A Photofragment Translational Spectroscopy Study Using Synchrotron Radiation for Product Photoionization," *J. Chem. Phys.* 108, 5784-5794 (1998).	CN,H,H_2,HCN Product Velocity Distributions $CH_2CHCN+h\nu$ Channels Dynamics Measurements
(77795)	Product Formation, Rate Constants, $CO_2^+ + e^-$ Dissociative Recombination	CO(d,e,a′),v,J
78169.	Ashfold, M.N.R., D.H. Mordaunt and S.H.S. Wilson, "High Resolution Photofragment Translational Spectroscopy of Hydride Molecules," *Comments At. Mol. Phys.* 32, 187-196 (1996).	C_2H,H NH_2,H Product Kinetic Energies $C_2H_2,NH_3+h\nu$ Dynamics
78170.	Kandel, S.A., T.P. Rakitzis, T. Lev-On and R.N. Zare, "Angular Distributions for the $Cl+C_2H_6 \rightarrow HCl+C_2H_5$ Reaction Observed via Multiphoton Ionization of the C_2H_5 Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2270-2273 (1998).	C_2H_5,C_3H_7 Product Kinetic Energy $Cl+C_2H_6,C_3H_8$ Spatial Anisotropy REMPI Probe
78171.	Lawruszczuk, R., M. Elhanine and B. Soep, "Selective Excitation of the Ion Pair Surface in the Intracluster Ca-HCl* Harpoon Reaction," *J. Chem. Phys.* 108, 8374-8380 (1998).	CaCl(X,v) Product State Distributions $Ca.HCl+h\nu$ P.E. Surfaces Dynamics Measurements
78172.	Rakitzis, T.P., S.A. Kandel and R.N. Zare, "Photolysis of ICl Causes Mass-Dependent Interference in the $Cl(^2P_{3/2})$ Photofragment Angular Momentum Distributions," *J. Chem. Phys.* 108, 8291-8294 (1998).	$Cl(^2P_{1/2,3/2})$ Product Angular Momentum Distributions $ICl+h\nu$
(78123)	Product Cross Sections, $F+D_2$, 2.07 kcal mol^{-1} Collision Energy, Crossed Beam Measurements	DF(v,J)

78173. Wong, T.H., C. Freel, P.D. Kleiber and K.M. Sando, "Scattering State Spectroscopy of the Reaction $Mg^*(3s3p^1P_1)+CH_4 \rightarrow MgH(v=0,1;N)+CH_3$," *J. Chem. Phys.* 108, 5723-5727 (1998).

MgH(v=0,1,N)
Product State Distributions
$Mg(^1P_1)+CH_4$
Quenching
Dynamics

78174. Akagi, H., Y. Fujimura and O. Kajimoto, "Vibrational State Distribution of Highly Vibrationally Excited $NO(X^2\Pi)$ Generated from the Reaction of $O(^1D)$ with N_2O," *J. Chem. Soc., Faraday Trans.* 94, 1575-1581 (1998).

NO(X,v=11-17)
Product State Distributions
$O(^1D)+N_2O$
NO(B,v=0-3)+M
Quenching
Rate Constants
$M=N_2,N_2O,O_2,O_3$

78175. Buijsse, B., W.J. van der Zande, A.T.J.B. Eppink, D.H. Parker, B.R. Lewis and S.T. Gibson, "Angular Distributions for Photodissociation of O_2 in the Herzberg Continuum," *J. Chem. Phys.* 108, 7229-7243 (1998).

$O(^3P_J)$
Product Angular Distributions
$O_2+h\nu$
Herzberg Continuum
Dynamics

78176. Fujiwara, H., and T. Ishiwata, "Doppler Spectroscopy of OH Fragments from the Photodissociation of HOCl at 266 and 355 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3856-3859 (1998).

OH
Kinetic Energies
$HOCl+h\nu$
Doppler Profiles
Dynamics

78177. Furuya, K., F. Koba and T. Ogawa, "Isotope Effects in Rovibrational Distributions of OH(A) and OD(A) Produced by Electron Impact on H_2O and D_2O," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 665-669 (1997).

OH,OD(A,v,J)
Product Distributions
H_2O,D_2O+e^-
17 eV Energy

78178. McCoy, A.B., M.W. Lufaso, M. Veneziani, S. Atrill and R. Naaman, "Reactions of Oxygen Atoms with van der Waals Complexes: The Effect of Complex Formation on the Internal Energy Distribution in the Products," *J. Chem. Phys.* 108, 9651-9657 (1998).

OH(J)
Product Energy Distributions
O+HCl.Ar
$O(^1D)$+HCl.Ar
Cluster Effects

78179. Wada, S.-i., and K. Obi, "Photochemical Reaction Dynamics of $O(^1D)$ with Saturated Hydrocarbons, CH_4, C_2H_6 and C_3H_8, Under Bulk Conditions and in van der Waals Complexes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3481-3491 (1998).

OH(v=0,1,J)
Product Distributions
$O(^1D)+CH_4,C_2H_6,C_3H_8$
$N_2O.RH+h\nu$
Comparisons
Cluster Effects

78180. Alagia, M., N. Balucani, L. Cartechini, P. Casavecchia, E.H. van Kleef, G.G. Volpi, P.J. Kuntz and J.J. Sloan, "Crossed Molecular Beams and Quasiclassical Trajectory Studies of the Reaction $O(^1D)+H_2(D_2)$," *J. Chem. Phys.* 108, 6698-6708 (1998).
OH,OD
Product Velocity Distributions
$O(^1D)+H_2,D_2$
Crossed Beams
Mechanism

(77806) Product Cross Sections, H^++O_2 Charge Exchange, Calculations
$O_2^+(v)$

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants and Section 40 for Reaction Dynamics)

78181. Maergoiz, A.I., E.E. Nikitin, J. Troe and V.G. Ushakov, "Classical Trajectory and Statistical Adiabatic Channel Study of the Dynamics of Capture and Unimolecular Bond Fission. IV. Valence Interactions Between Atoms and Linear Rotors," *J. Chem. Phys.* 108, 5265-5280 (1998).
Unimolecular Rate Theory
A+BC
Capture
Rate Constants
Analytical Forms

78182. Kato, T., "Nonequilibrium Unimolecular Dissociation Influenced by Intramolecular Vibrational Energy Redistribution," *J. Chem. Phys.* 108, 6611-6618 (1998).`
Unimolecular Dissociation
Slow IVR
Nonequilibrium
Generalized Theory

78183. Reid, S.A., and H. Reisler, "Experimental Studies of Resonances in Unimolecular Decomposition," *Ann. Rev. Phys. Chem.* 47, 495-525 (1996).
Unimolecular Photodissociation
CH_3O,HCO,
HFCO,NO_2
Review

78184. Reisler, H., and C. Wittig, "State Resolved Simple Bond Fission Reactions: Experiment and Theory," in *Advances in Chemical Kinetic and Dynamics*, J.R. Barker, ed., 5 Reviews, 280 pp., Volume 1, 139-185 (1992).
Unimolecular Bond Fission
t-$C_4H_9NO+h\nu$
$NCNO+h\nu$
RRKM Theory
Review

78185. Wesolowski, S.S., J.M. Galbraith and H.F. Schaefer III, "Isomerization Pathway of the Aluminum Monocarbonyl/Isocarbonyl Pair, AlCO/AlOC: Evidence of a Cyclic Minimum," *J. Chem. Phys.* 108, 9398-9403 (1998).
Isomerization
AlCO/AlOC
Energy Barriers
Cyclic Isomer Role
Theory

78186.	Yamaguchi, Y., S.S. Wesolowski, T.J. Van Huis and H.F. Schaefer III, "The Unimolecular Dissociation of H_2CO on the Lowest Triplet Potential Energy Surface," *J. Chem. Phys.* 108, 5281-5288 (1998).	Unimolecular Dissociation CH_2O Triplet Surface Energy Barriers
78187.	Jursic, B.S., "Density Functional Theory Study of Difluorovinylidene Isomerization to Difluoroacetylene," *Int. J. Quantum Chem.* 62, 515-520 (1997).	Isomerization CCF_2/FCCF Transition State Energy Barrier DFT Calculations
78188.	Breidung, J., H. Burger, C. Kotting, R. Kopitzky, W. Sander, M. Senzlober, W. Thiel and H. Willner, "Difluorovinylidene, $F_2C=C$," *Angew. Chem. Int. Ed. Engl.* 36, 1983-1985 (1997).	Isomerization CF_2C/C_2F_2 Barrier Photoinduced IR Spectra Matrix Study
78189.	Shibata, T., H. Li, H. Katayanagi and T. Suzuki, "Dissociation of Metastable CH_3CO Radical Observed by Subpicosecond Time-Clocked Photofragment Imaging," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3643-3647 (1998).	Unimolecular Dissociation $CH_3COCl + h\nu$ CH_3CO Fragment Sub ps Probe Ion Imaging
78190.	Ferguson, H.A., J.D. Ferguson and B.E. Holmes, "Threshold Energies and Unimolecular Rate Constants for Elimination of HF from Chemically Activated $CF_3CH_2CH_3$ and $CF_3CH_2CF_3$: Effect of CH_3 and CF_3 Substituents at the β-Carbon and Implications about the Transition State," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5393-5397 (1998).	Unimolecular Dissociation $CF_3C_2H_5$ $CF_3CH_2CF_3$ HF Elimination Rate Constants Threshold Energies
(78321)	Isomerization, Structural Calculations, Energies, Geometries	C_3H_3O
78191.	Doslic, N., O. Kuhn and J. Manz, "Infrared Laser Pulse Controlled Ultrafast H-Atom Switching in Two-Dimensional Asymmetric Double Well Potentials," *Ber. Bunsenges. Phys. Chem.* 102, 292-297 (1998).	Isomerization CH(OH)CHCHO H-Atom Transfer Laser Induced Model
78192.	Dubnikova, F., and A. Lifshitz, "Structural and Geometrical Isomerizations of Cyclopropane: Quantum Chemical and RRKM Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3299-3306 (1998).	Isomerization *c*-C_3H_6/C_3H_6 Transition States DFT/RRKM Calculations

78193.	Owrutsky, J.C., and A.P. Baronavski, "Ultrafast Studies of the Photodissociation of the Acetone 3s Rydberg State at 195 nm: Formation and Unimolecular Dissociation of the Acetyl Radical," *J. Chem. Phys.* 108, 6652-6659 (1998).	Unimolecular Dissociation $(CH_3)_2CO$ Rydberg States CH_3CO ps Time Resolution RRKM Analysis
78194.	Gershinsky, G., and E. Pollak, "Isomerization of *trans*-Stilbene: Theory for Pressure Dependence of the Rate," *J. Chem. Phys.* 108, 9186-9187 (1998).	Isomerization $(C_6H_5CH)_2/M$ $M=CH_4, C_2H_6$ Pressure Dependence Theory
78195.	Stogner, S.M., and R.S. Grev, "Germyne, H-C≡Ge-H, and the Excited States of 1-Germavinylidene, $H_2C=Ge$," *J. Chem. Phys.* 108, 5458-5464 (1998).	Isomerization $GeCH_2/GeHCH$ Barriers Stabilities Calculations
(78342)	Isomerization Energy Barriers, Geometries, Frequencies Structural Calculations	NH_3NH
78196.	Smirnov, V.N., "A Study of Transient Processes in Unimolecular Reactions within the Framework of the Modified Exponential Model of the Collisional Transition Probability Density," *Kinet. Catal., Russia* 38, 147-154 (1997).	Unimolecular Dissociation New Model N_2O
78197.	Smirnov, V.N., "RRKM Analysis of Two Channel Decomposition of Si_2H_6," *Kinet. Catal., Russia* 38, 309-320 (1997).	Unimolecular Dissociation Si_2H_6/SiH_4+SiH_2 $Si_2H_6/Si_2H_4+H_2$ High Pressure Rate Constants RRKM Analysis

40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

78198.	Malick, D.K., G.A. Petersson and J.A. Montgomery Jr, "Transition States for Chemical Reactions. I. Geometry and Classical Barrier Height," *J. Chem. Phys.* 108, 5704-5713 (1998).	Reaction Dynamics Transition States Barrier Height Calculations New Procedure

78199. Bowman, J.M., and G.C. Schatz, "Theoretical Studies of Polyatomic Bimolecular Reaction Dynamics," *Ann. Rev. Phys. Chem.* 46, 169-195 (1995).

Reaction Dynamics
B,Cl + H_2O
CH + N_2
CN + HCl,H_2,OH
H + C_2H_2,HCN
Cl,O + HCN
O + Cl_2
OH + CH_4,HBr,HCl
OH + H_2,HD,D_2
Theoretical Methods,Review

78200. Donahue, N.M., J.S. Clarke and J.G. Anderson, "Predicting Radical-Molecule Barrier Heights: The Role of the Ionic Surface,"*J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3923-3933 (1998).

Reaction Dynamics
F,Cl,Br + Alkanes
H,O,OH + Alkanes
Barrier Heights
Curve Crossing
Theoretical Method

78201. Marchand, N., J.C. Rayez and S.C. Smith, "Theoretical Study of the Reaction CH($X^2\Pi$) + NO($X^2\Pi$). III. Determination of the Branching Ratios," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3358-3367 (1998).

Reaction Dynamics
CH + NO
Channels
Branching Ratios
T Dependence

78202. Jursic, B.S., "Computational Studies of Formaldehyde Dissociation and Protonated Carbon Monoxide Isomerization with Density Functional Theory Methods," *J. Mol. Struct.* 418, 11-16 (1997).

Reaction Dynamics
CH_2O/CO + H_2
H^+CO/HCO^+
Isomerization
Energies,Barriers

78203. Anglada, J.M., J.M. Bofill, S. Olivella and A. Sole, "Theoretical Investigation of the Low-lying Electronic States of Dioxirane: Ring Opening to Dioxymethane and Dissociation into CO_2 and H_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3398-3406 (1998).

Reaction Dynamics
c-CH_2O_2/CO_2 + H_2
Low-lying States
Ring Opening/ Dissociation
Energies

78204. Pilling, M.J., "Radical-Radical Reactions," *Ann. Rev. Phys. Chem.* 47, 81-108 (1996).

Reaction Dynamics
Radical/Radical Reactions
CH_3 + CH_3,H,OH
Transition States
Review

78205. Hessler, J.P., "Calculation of Reactive Cross Sections and Microcanonical Rates from Kinetic and Thermochemical Data," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4517-4526 (1998).

Reaction Dynamics
CH_3 + CH_3/C_2H_6
H + O_2/OH + O
Transformed
Energy Dependent
Cross Sections
Descriptions

78206. Bu, Y., Y. Ding and C. Deng, "Ab Initio Time-Dependent Perturbation Study of Tunneling Effect in the Abstraction of Hydrogen from Methane by Methyl Radical," *J. Mol. Struct.* 417, 69-80 (1997).

Reaction Dynamics
$CH_3 + CH_4$
H Abstraction
Tunneling
Probabilities

78207. Wong, M.W., and L. Radom, "Radical Addition to Alkenes: Further Assessment of Theoretical Procedures," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2237-2245 (1998).

Reaction Dynamics
CH_3 + Alkenes
CH_2OH + Alkenes
CH_2CN + Alkenes
Energy Barriers
$\Delta H_{Reaction}$

78208. Korchowiec, J., and T. Uchimaru, "Density Functional Study of Addition of Fluoromethyl Radicals to Fluoroethylenes: Estimation of Activation Energies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2439-2442 (1998).

Reaction Dynamics
$CH_3, CH_2F + C_2H_{4-n}F_n$
$CHF_2, CF_3 + C_2H_{4-n}F_n$
$n = 0\text{-}4$
Activation Energies

78209. Corchado, J.C., E.L. Coitino, Y.-Y. Chuang, P.L. Fast and D.G. Truhlar, "Interpolated Variational Transition State Theory by Mapping," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2424-2438 (1998).

Reaction Dynamics
$CH_3 + H_2$
$OH + CH_4, H_2$
$Cl^- + CH_3Cl$
$HBr + C_2H_2$
C_5H_8
Rate Constants
VTST
New Algorithms

78210. Mestres, J., and P.C. Hiberty, "Quantitative Valence Bond Computations of Curve Crossing Diagrams for a Hydride-Transfer Model Reaction: $CH_4 + CH_3^+ \rightarrow CH_3^+ + CH_4$," *New J. Chem.* 20, 1213-1219 (1996).

Reaction Dynamics
$CH_3^+ + CH_4$
H-Transfer
Curve Crossing
Mechanism

78211. Tapia, O., V. Moliner and J. Andres, "A Quantum Electronic Theory of Chemical Processes. The Inverted Energy Profile Case: $CH_3^+ + H_2$ Reaction," *Int. J. Quantum Chem.* 63, 373-391 (1997).

Reaction Dynamics
$CH_3^+ + H_2$
D Substitution
Transition States

78212. Politzer, P., J.M. Seminario, M.C. Concha and A.G. Zacarias, "Density Functional Investigation of Some Decomposition Routes of Methyl Nitrate," *Int. J. Quantum Chem.* 64, 205-210 (1997).

Reaction Dynamics
CH_3ONO_2
Dissociation Channels
DFT Energies

78213. Zhu, W., J.Z.H. Zhang and D.H. Zhang, "Full-Dimensional Quantum Dynamics Calculation for D_2+CN Reaction," *Chem. Phys. Lett.* 292, 46-50 (1998).

Reaction Dynamics
$CN + D_2$
P.E. Surface
Rate Constants
Calculations

78214. Rice, B.M., and C.F. Chabalowski, "Addendum - Ab Initio Potential Energy Surface for H+OCS Reactions: Extended Basis Sets and Correlation Treatment," [*J. Phys. Chem.* 98, 9488-9497 (1994)]," *ibid.* A102, 3847 (1998).

Reaction Dynamics
COS+H
P.E. Surface
Energy Barriers
Addendum

78215. Il'chenko, N.N., Yu.A. Serguchev, L.G. Gorb and R.B. Gutsulyak, "Ab Initio Quantum Chemical Calculation of the Mechanism for Molecular Addition of Chlorine to Acetylene in the Gas Phase," *Theor. Exp. Chem., Russia* 32, 17-19 (1996).

Reaction Dynamics
$C_2H_2+Cl_2$
TS Structures
Mechanism

78216. Ha, T.-K., J. Pochert and M. Quack, "Ab Initio Calculations of the Structure, Kinetics and Infrared Laser Chemical Reaction Dynamics of Fluorooxirane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5241-5252 (1998).

Reaction Dynamics
c-$C_2H_3F(O)$
P.E. Surfaces
Dissociation
Channels

78217. Frank, I., M. Parrinello and A. Klamt, "Insight into Chemical Reactions from First Principles Simulations: The Mechanism of the Gas Phase Reaction of OH Radicals with Ketones," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3614-3617 (1998).

Reaction Dynamics
$C_2H_5COC_3H_7+OH$
Channels
Ring TS Role

78218. Roberto-Neto, O., E.L. Coitino and D.G. Truhlar, "Dual-Level Direct Dynamics Calculations of Deuterium and Carbon-13 Kinetic Isotope Effects for the Reaction $Cl+CH_4$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4568-4578 (1998).

Reaction Dynamics
$Cl+CH_4$
Rate Constants
Isotopic Effects

78219. Filatov, M., and S. Shaik, "Theoretical Investigation of Two-State-Reactivity Pathways of H-H Activation by FeO^+: Addition-Elimination, Rebound, and Oxene-Insertion Mechanisms," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3835-3846 (1998).

Reaction Dynamics
FeO^++H_2
DFT Calculations
Channels
Excited State
Effects

78220. Lee, W.T., and R.I. Masel, "Ab Initio Tests of the Marcus Equation for the Prediction of the Position of the Transition State for the Reaction $H+C_2H_5R \rightarrow CH_4+CH_2R$ with R=H, CH_3, NH_2, CN, CF_3 and C_6H_5," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2332-2341 (1998).

Reaction Dynamics
$H+C_2H_5R$
CH_4 Product Channel
TS Prediction
Limitations

78221. Bradley, K.S., and G.C. Schatz, "A Quasiclassical Trajectory Study of $H+H_2O \rightarrow OH+H_2$: Angular Distributions and OH Angular Momentum Alignment," *J. Chem. Phys.* 108, 7994-8003 (1998).

Reaction Dynamics
$H+H_2O$
OH,H_2 Product
Distributions
Mechanisms

78222. Meijer, A.J.H.M., and E.M. Goldfield, "Time-Dependent Quantum Mechanical Calculations on $H+O_2$ for Total Angular Momentum J>0," *J. Chem. Phys.* 108, 5404-5413 (1998).

Reaction Dynamics
$H+O_2(J)$
Probabilities
Rotational
Effects

78223. Groenenboom, G.C., "Discrete Variational Quantum Reactive Scattering Method with Optimal Distorted Waves. II. Application to the Reaction $H+O_2 \rightarrow OH+O$," *J. Chem. Phys.* 108, 5677-5682 (1998).

Reaction Dynamics
$H+O_2(v,J)$
Probabilities
Variational Method

78224. Gu, J., Y. Xie and H.F. Schaefer III, "The Barrier Height for Decomposition of HN_2," *J. Chem. Phys.* 108, 8029-8030 (1998).

Reaction Dynamics
$HN_2/H+N_2$
Exothermicity
Barrier Height
$DeNO_x$ Kinetics

78225. Sumathi, R., and S.D. Peyerimhoff, "Theoretical Investigations on the Reactions $NH+HO_2$ and NH_2+O_2: Electronic Structure Calculations and Kinetic Analysis," *J. Chem. Phys.* 108, 5510-5521 (1998).

Reaction Dynamics
$NH+HO_2$
NH_2+O_2
Rate Constants
Channels

78226. Sumathi, R., D. Sengupta and M.T. Nguyen, "Theoretical Study of the H_2+NO and Related Reactions of $[H_2NO]$ Isomers," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3175-3183 (1998).

Reaction Dynamics
$NH+OH$
NH_2+O
$H+HNO$
$NO+H_2$
Rate Constants
TS Energies
$\Delta H_f(NH_2O,HNOH)$

78227. Moskaleva, L.V., and M.C. Lin, "Theoretical Study of the $NH_2+C_2H_2$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4687-4693 (1998).

Reaction Dynamics
$NH_2+C_2H_2$
Rate Constants
Channels
RRKM Analysis
P.E. Surfaces

78228. Polak, R., I. Paidarova and P.J. Kuntz, "On the Fragmentation Dynamics of $NH_3 \rightarrow NH_2+H$. II. Diatomics-in-Molecules Potential Energy Surfaces," *Int. J. Quantum Chem.* 62, 659-667 (1997).

Reaction Dynamics
NH_3/NH_2+H
P.E. Surfaces
DIM Model

78229. Kulkarni, S.A., and N. Koga, "Ab Initio Density Functional Investigation of Reactions of NO with XCO(X=H,F,Cl)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5228-5235 (1998).

Reaction Dynamics
NO+HCO
NO+FCO
NO+ClCO
Channels
RRKM Rate Constants

78230. Gargano, R., S. Crocchianti, A. Lagana and G.A. Parker, "The Quantum Threshold Behavior of the Na+HF Reaction," *J. Chem. Phys.* 108, 6266-6271 (1998).

Reaction Dynamics
Na+HF(v)
Probabilities
NaF(v,J) Product Distributions
Energy Effects

78231. Topaler, M.S., D.G. Truhlar, X.Y. Chang, P. Piecuch and J.C. Polanyi, "The Photoabsorption Spectrum of Na···FH van der Waals Molecule: Comparison of Theory and Experiment for a Harpooning Reaction Studied by Transition State Spectroscopy," *J. Chem. Phys.* 108, 5378-5390 (1998).

Reaction Dynamics
Na.FH + hν
Low-lying Surfaces
Reactive/
E-V Transfer
Channels
Theory/Experiment
Comparisons

78232. Corchado, J.C., J. Espinosa-Garcia, O. Roberto-Neto, Y.-Y. Chuang and D.G. Truhlar, "Dual-Level Direct Dynamics Calculations of the Reaction Rates for a Jahn-Teller Reaction: Hydrogen Abstraction from CH_4 or CD_4 by $O(^3P)$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4899-4910 (1998).

Reaction Dynamics
$O+CD_4$
$O+CH_4$
Rate Constants
T Dependences
VTST

78233. Yarkony, D.R., "On the Mechanism of the Spin-Nonconserving Chemical Reaction $O(^3P)+HCCH \rightarrow CH_2(a^1A_1)+CO(X^1\Sigma^+)$. I. Feasibility," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5305-5311 (1998).

Reaction Dynamics
$O+C_2H_2$
Spin Forbidden
CH_2(a),CO(X)
Product Channel
P.E. Surfaces
Energies

78234. Perdih, M., I.W.M. Smith and A. Miklavc, "Kinematic Mass Model of Activated Bimolecular Reactions: Reactions of Vibrationally Excited Reactants," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3907-3915 (1998).

Reaction Dynamics
O+DCl(v=1)
O+HCl(v=1)
$O+H_2(v=1)$
Cross Sections
Calculation Method

78235. Poirier, B., "Quantum Reactive Scattering for Three-Body Systems via Optimized Preconditioning, as Applied to the O+HCl Reaction," *J. Chem. Phys.* 108, 5216-5224 (1998).

Reaction Dynamics
O+HCl
Probabilities
Rate Constants
Preconditioning
Method

78236. Tolstikhin, O.I., and H. Nakamura, "Hyperspherical Elliptic Coordinates for the Theory of Light Atom Transfer Reactions in Atom-Diatom Collisions," *J. Chem. Phys.* 108, 8899-8921 (1998).

Reaction Dynamics
O+HCl
H-Atom Transfer
Probabilities
New Method

78237. Nobusada, K., O.I. Tolstikhin and H. Nakamura, "Quantum Mechanical Elucidation of Reaction Mechanisms of Heavy-Light-Heavy Systems: Role of Potential Ridge," *J. Chem. Phys.* 108, 8922-8930 (1998).

Reaction Dynamics
O+HCl
H-Atom Transfer
Probabilities
Product State
Energies

78238. Skinner, D.E., T.C. Germann and W.H. Miller, "Quantum Mechanical Rate Constants for $O+OH \leftrightarrow H+O_2$ for Total Angular Momentum J>0," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3828-3834 (1998).

Reaction Dynamics
$O+OH/$
$H+O_2$
Rate Constants

78239. Aliagas, I., and S. Gronert, "Accuracy of G2 Calculations for the Reactions of Hydroxyl Radicals with Alkanes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2609-2612 (1998).

Reaction Dynamics
$OH+CH_4,C_2H_6$
$OH+C_3H_8,C_4H_{10}$
Activation Energies

78240. Matzkies, F., and U. Manthe, "Accurate Quantum Calculations of Thermal Rate Constants Employing MCTDH: $H_2+OH \rightarrow H+H_2O$ and $D_2+OH \rightarrow D+DOH$," *J. Chem. Phys.* 108, 4828-4836 (1998).

Reaction Dynamics
$OH+D_2$
$OH+H_2$
Rate Constants
Improved Method

78241. Jursic, B.S., "The Computation of the Potential Energy Surface for $H_2+OH \rightarrow H_2O+H$ Using ab Initio and Density Functional Theory Methods," *Int. J. Quantum Chem.* 62, 639-644 (1997).

Reaction Dynamics
$OH+H_2/$
H_2O+H
P.E. Surface
Energetics
TS Geometries

78242. Liwo, A., D. Dyl, D. Jeziorek, M. Nowacka, T. Ossowski and W. Woznicki, "MCSCF Study of Singlet Oxygen Addition to Ethenol: A Model of Photooxidation Reactions of Unsaturated and Aromatic Compounds Bearing Hydroxy Groups," *J. Computat. Chem.* 18, 1668-1681 (1997).

Reaction Dynamics
$O_2(a)+C_2H_3OH$
Channels
TS Energies

78243. Castillo, S., A. Cruz, V. Bertin, E. Poulain, J.S. Arellano and G. Del Angel, "Theoretical Study on Pd Dimer and Trimer Interaction with the Hydrogen Molecule," *Int. J. Quantum Chem.* 62, 29-45 (1997).

Reaction Dynamics
Pd_2+H_2
Pd_3+H_2
P.E. Surfaces
Low-lying States

78244. Cui, Q., D.G. Musaev and K. Morokuma, "Molecular Orbital Study of H_2 and CH_4 Activation on Small Metal Clusters. I. Pt, Pd, Pt_2 and Pd_2," *J. Chem. Phys.* 108, 8418-8428 (1998).

Reaction Dynamics
Pt,Pt_2+CH_4,H_2
Pd,Pd_2+CH_4,H_2
Channels
Reactivities
Energetics
Calculations

78245. Bishenden, E., and D.J. Donaldson, "Ab Initio Study of SO_2+H_2O," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4638-4642 (1998).

Reaction Dynamics
SO_2+H_2O/H_2SO_3
$SO_2+H_2O/SO_2.H_2O$
Channel Energetics
Thermochemistries
Gas/Aqueous Phases

78246. Irigoras, A., J.E. Fowler and J.M. Ugalde, "Erratum - On the Reactivity of $Ti^+(^4F,^2F)$: Reaction of Ti^+ with OH_2 [*J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 293-300 (1998)]," *ibid.* 2252.

Reaction Dynamics
$Ti^+ + H_2O$
Channels
Energies
Erratum

41. CHEMICAL KINETICS - GENERAL

(See also Section 42 for Laser Controlled Kinetics)

78247. Temkin, O.N., A.V. Zeigarnik and D. Bonchev, *"Chemical Reaction Networks: A Graph-Theoretical Approach,"* 286 pp., 5 Chapters, CRC Press, Boca Raton FL (1996).

Chemical Reaction
Mechanisms
Graph Theory
Combinatorics
Approaches
Monograph

(78079) Combustion Kinetics, Modeling Needs, Review

Chain Mechanisms

78248. Scott, S.K., "Global Behavior in the Oxidation of Hydrogen, Carbon Monoxide and Simple Hydrocarbons," Chapter 5 in *Low Temperature Combustion and Autoignition*, M.J. Pilling, ed., 7 Chapters, 794 pp., *Comprehensive Chemical Kinetics* 35, 439-544 (1997).

Kinetic
Oscillations
$CO,H_2/O_2$
$Hydrocarbons/O_2$
Ignition
Nonlinear
Mathematics
Review

(77715)
(77716) CO/O_2 Catalytic Oxidation, Model

Kinetic
Oscillations

(77827) Catalytic Reduction of NO_x by C_3H_6/Pt/V Zeolites, H_2O Effects

Kinetic
Oscillations

(77828) N_2O/Cu Zeolite Catalytic Dissociation, N_2O Outlet Variations, O_2 Effects

Kinetic
Oscillations

78249. Ionikh, Yu.Z., I.N. Kostyukevich and N.V. Chernysheva, "Concentration of C_2 Molecules and the Kinetics of Their Formation and Destruction in a Glow Discharge in a He/CO Mixture," *Opt. Spectrosc., Russia* 80, 527-531 (1996).

$C_2(d,A)$
Formation
CO/He Discharge
Densities
E-E Transfer

(77870) C_6H_6 Formation, Jet Stirred Reactor

$C_2H_2,C_3H_4/O_2$
$C_3H_6,C_4H_6/O_2$

78250. Tuazon, E.C., S.M. Aschmann, R. Atkinson and W.P.L. Carter, "The Reactions of Selected Acetates with the OH Radical in the Presence of NO: Novel Rearrangement of Alkoxy Radicals of Structure RC(O)OCH(O)R," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2316-2321 (1998).

$CH_3COOR+OH/NO$
$R=C_1$-C_4 Alkyl
Product Yields
Mechanisms

78251. Arrington, C.A., C. Ramos, A.D. Robinson and T.S. Zwier, "Aromatic Ring-Forming Reactions of Metastable Diacetylene with 1,3-Butadiene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3315-3322 (1998).

$^3C_4H_2^*+C_4H_6$
Mass Analysis
C_6H_6 ,C_8H_6
Ring Forming Products

78252. Ciajolo, A., A. D'Anna and M. Kurz, "Low Temperature Oxidation of Methyl *tert*-Butyl Ether in a High Pressure Jet-Stirred Flow Reactor," *Combust. Sci. Technol.* 123, 49-61 (1997).

t-$C_4H_9OCH_3/O_2$
Jet Stirred Flow Reactor
Product Analysis
Engine End-Gas Conditions

(78099) Pyrolysis and Oxidation Reaction Mechanisms

n-C_7H_{16}/O_2

78253. Dagaut, P., R. Koch and M. Cathonnet, "The Oxidation of *n*-Heptane in the Presence of Oxygenated Octane Improvers MTBE and ETBE," *Combust. Sci. Technol.* 122, 345-361 (1997).

n-C_7H_{16}/O_2
MTBE,ETBE
Jet Stirred Reactor
Additive Effects

78254. Brezinsky, K., and C.R. Shaddix, "The Power of Analogies in Chemical Kinetics," pp. 87-104 in *Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman*, F.L. Dryer and R.F. Sawyer, eds., 505 pp., 17 Papers Presented at a Colloquium Held at Princeton NJ, October 1993, Gordon and Breach Science Publishers, Amsterdam, The Netherlands (1997).

$C_{10}H_8/O_2$
Oxidation Mechanism
Aromatic Similarities

78255. Dubey, M.K., M.P. McGrath, G.P. Smith and F.S. Rowland, "HCl Yield from OH+ClO: Stratospheric Model Sensitivities and Elementary Rate Theory Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3127-3133 (1998).

ClO+OH
HCl Product Yields
Calculations

78256. Otorbaev, D.K., M.J. de Graaf, M.C.M. van de Sanden and D.C. Schram, "Vibrational Population of Hydrogen Molecules Excited by a Radiofrequency Discharge in an Expanding Thermal Arc Plasma as Determined by Emission Spectroscopy," *Contrib. Plasma Phys.* 35, 195-202 (1995).

$H_2(v)$
Populations
H_2 RF Discharge

78257. Jost, R., "Magnetic Field Control of Molecular Dissociation Energies," *Int. J. Quantum Chem.* 64, 571-580 (1997).

Molecular Dissociation
NO_2
Magnetic Field
Energy
Controlling Effects

(77889) Back Corona Discharge Method

NO_2/N_2
Dissociation

78258. Jacobs, H., F. Miethke, A. Rutscher and H.-E. Wagner, "Reaction Kinetics and Chemical Quasi-Equilibria of the Ozone Synthesis in Oxygen DC Discharges," *Contrib. Plasma Phys.* 36, 471-486 (1996).

O_3 Formation
O_2 DC Discharge
Species Profiles
Kinetic Modeling
$O_2(a)$ Role

42. LASERS/INDUCED EFFECTS/MPI

78259.	Sola, I.R., J. Santamaria and D.J. Tannor, "Optimal Control of Multiphoton Excitation: A Black Box or a Flexible Toolkit?," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4301-4309 (1998).	Reaction Control fs IR MPA Methods
78260.	Kawashima, H., M.M. Wefers and K.A. Nelson, "Femtosecond Pulse Shaping, Multiple-Pulse Spectroscopy and Optical Control," *Ann. Rev. Phys. Chem.* 46, 627-656 (1995).	fs Spectroscopy Laser Pulse Shaping Methods Review
(78191)	CH(OH)CHCHO, H-Transfer, Model	Laser Induced Isomerization
78261.	Ivanov, G.K., and G.V. Golubkov, "Elementary Reactions in a Field of Monochromatic Laser Radiation," *Chem. Phys. Reports* 16, 1001-1011 (1997).	Laser Control $Cl+H_2$ Field Induced Resonances
(77803)	Laser Control, Photoionization, fs 2-Pulse Method	Cs_2(B)
78262.	Gronager, M., and N.E. Henriksen, "Real-Time Control of Electronic Motion: Application to HD^+," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4277-4283 (1998).	Reaction Control $HD^+ + h\nu$ D^+,D Product Branching IR fs Laser Pulse Method
78263.	Uberna, R., M. Khalil, R.M. Williams, J.M. Papanikolas and S.R. Leone, "Phase and Amplitude Control in the Formation and Detection of Rotational Wavepackets in the $E^1\Sigma_g^+$ State of Li_2," *J. Chem. Phys.* 108, 9259-9274 (1998).	Wavepacket fs Laser Control Li_2(E,v,J) Formation/ Detection Method
(77924)	BC_2H_n, n=1-5, FTIR Product Analysis, Matrix Study	Laser Ablation B/C_2H_4,C_2H_6
(77950)	CoN, NiN, $(CoN)_2$, $(NiN)_2$ Product FTIR Spectra, Frequencies, Matrix Study	Laser Ablation Co,Ni/N_2
(78062)	Mass Analysis, M^+, MO^+ Plumes	Laser Ablation Lanthanides
(77994)	ThN, ThN_2, UN, UN_2, Product FTIR Analysis, Matrix Study	Laser Ablation Th,U/N_2
(78061)	Atomic Analysis, Detection Limits, Methods, Review	Laser Induced Ionization

78264. Ledingham, K.W.D., R.P. Singhal, D.J. Smith, T. McCanny, P. Graham, H.S. Kilic, W.X. Peng, S.L. Wang, A.J. Langley, P.F. Taday and C. Kosmidis, "Behavior of Polyatomic Molecules in Intense Infrared Laser Beams," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3002-3005 (1998).
IR MPI
fs Laser Pulses
Polyatomics
Parent Ions

78265. Poth, L., and A.W. Castleman Jr, "Molecular Dynamics Simulation of Coulomb Explosion Processes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4075-4081 (1998).
MPI
Clusters
Ar_n,$(CH_3COCH_3)_n$
fs Pulses
Product Ion Energies

(78170) C_2H_6, C_3H_8+Cl, Product Kinetic Energies, Spatial Anisotropy
REMPI
C_2H_5,C_3H_7

(78148) MPD/MPI, fs Laser Pulses, Ion Yields
C_6H_6,C_6H_8
C_6H_{12},C_6H_{14}

(78063) REMPI/Mass Analysis Monitor, CH_4/O_2/Ar Diffusion Flame
$C_{10}H_8$,$C_{13}H_{10}$
$C_{14}H_{10}$,PAHS

(78152) MPI, Fragmentation Product Patterns
$Cr(CO)_6$
$Cr(CO)_6.(CH_3OH)_n$

78266. Banares, L., T. Baumert, M. Bergt, B. Kiefer and G. Gerber, "The Ultrafast Photodissociation of $Fe(CO)_5$ in the Gas Phase," *J. Chem. Phys.* 108, 5799-5811 (1998).
MPI
$Fe(CO)_5$
fs Laser Pulses
Fragment Ion Patterns

(77952) R2PI Spectra, Rg=Ar,Kr,Xe, Constants, D_0', D_0''
GaRg(F,G,H,I)

(77961) 2-Color REMPI, Mass Analysis, Perturbing A-State Vibrational Levels
HgAr(B-X)

(77971) LIF/REMPI Spectral Measurements, Theoretical Interpretations
NO.Ar(D,C,A-X)

(77972) REMPI Spectra, Rg^+ Formation
NO.Ar;NO.Kr
NO.Xe

78267. Ivanov, G.K., D.M. Manakov and G.V. Golubkov, "Multiphoton Ionization of Atoms via a Series of Intermediate Rydberg States," *Chem. Phys. Reports* 16, 1013-1023 (1997).
MPI
Na
Rydberg State Role

43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects and Section 40 for Surface Dynamics)

78268.	Leach, C.A., and R.E. Moss, "Spectroscopy and Quantum Mechanics of the Hydrogen Molecular Cation: A Test of Molecular Quantum Mechanics," *Ann. Rev. Phys. Chem.* 46, 55-82 (1995).	Energy Levels H_2^+,HD^+,D_2^+ Near Limit Spectroscopy Theory/Experiment Review
78269.	Csaszar, A.G., and I.M. Mills, "Vibrational Energy Levels of Water," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 1101-1122 (1997).	Vibrational Energy Levels H_2O ≤ 1500 cm^{-1} Isotopomers Calculations
78270.	Kirmse, B., A. Delon and R. Jost, "The NO_2 Vibronic Levels Near the (X^2A_1-A^2B_2) Conical Intersection Observed by Laser Induced Dispersed Fluorescence," *J. Chem. Phys.* 108, 6638-6651 (1998).	Vibrational Energy Levels NO_2(A-X) LIF Conical Intersection A/X Mixing
78271.	Vilanove, H., and M. Jacon, "Discrete Variable Representation Method Applied to the Determination of Rotation-Vibration Bound States of NO_2," *Int. J. Quantum Chem.* 62, 199-211 (1997).	v,J Energy Levels NO_2 $v \leq 5, J \leq 11$ Calculation Method
78272.	Li, J., Y. Liu, H. Chen, H. Gao, J. Xiang, D. Chen, G. Wu, L. Li and R.W. Field, "Predissociation of the $Na_2(4^3\Sigma_g^+)$ State," *J. Chem. Phys.* 108, 7707-7712 (1998).	$Na_2(4^3\Sigma_g^+)$ Predissociative Vibrational Levels P.E. Curve OODR Measurements
78273.	Gosper, J.J., and C. McMenamin, "GRIDVIEW: A Windows Program for Visualization of Potential Energy Surfaces," *J. Mol. Struct.* 419, 37-50 (1997).	P.E. Surfaces Visualization Software
78274.	Wang, H., and W.C. Stwalley, "Ultracold Photoassociative Spectroscopy of Heteronuclear Alkali Metal Diatomic Molecules," *J. Chem. Phys.* 108, 5767-5771 (1998).	P.E. Curves Mixed Alkali Dimers 10 MM′ Cases Long Range Free/Bound F.C. Factors

78275. Lievin, J., and N. Vaeck, "Use of Symmetry-Adapted Brillouin Theorem to Analyze the Variational Content of Molecular Wave Functions Along Potential Energy Surfaces: Application to BH_2 and PO_2," *Int. J. Quantum Chem.* 62, 521-541 (1997).

P.E. Surfaces
BH_2,PO_2
Appropriate Theoretical Descriptions

78276. Gordon, M.S., V.-A. Glezakou and D.R. Yarkony, "Systematic Location of Intersecting Seams of Conical Intersection in Triatomic Molecules: The ($1^2A'$-$2^2A'$) Conical Intersections in BH_2," *J. Chem. Phys.* 108, 5657-5659 (1998).

P.E. Surfaces
$BH_2(2,1^2A')$
Conical Intersection Seam Location

78277. Alekseyev, A.B., H.-P. Liebermann, G. Hirsch and R.J. Buenker, "Relativistic Configuration Interaction Calculations of the Potential Curves and Radiative Lifetimes of the Low-lying States of Bismuth Nitride," *Chem. Phys.* 225, 247-258 (1997).

P.E. Curves
BiN
Low-lying States
Spectral Constants
Transition Probabilities
Lifetimes
Calculations

(78303) P.E. Surfaces, Frequencies, (B-X) Spectral Assignments, Structural Calculations

CHO,CDO(B,X)

(78171) P.E. Surfaces, Dynamics, CaCl(X,v) Product State Distributions, Measurements

Ca.HCl+hν

78278. Fiedler, A., and S. Iwata, "Variety of [Fe,N,O] Isomers: A Theoretical Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3618-3624 (1998).

P.E. Surfaces
FeNO
Isomers
Geometries

(78124) Reactive Cross Section Measurements, P.E. Surface Calculation Accuracies

$H+D_2$

78279. Koput, J., and S. Carter, "The Potential Energy Surface and Vibrational-Rotational Energy Levels of HCP," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 1091-1100 (1997).

P.E. Surface
HCP
v,J Energy Levels
Spectral Constants
Calculations

78280. Fang, W.-H., M. Peric and S.D. Peyerimhoff, "Ab Initio Study of the Potential Energy Surfaces for the Valence and Rydberg Doublet Electronic States of HNF," *Chem. Phys.* 223, 119-129 (1997).

P.E. Curves
HNF
Low-lying Doublet States

78281. Peterson, K.A., "Accurate ab Initio Near-Equilibrium Potential Energy and Dipole Moment Functions of HOCl and HOBr," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 1051-1064 (1997).

P.E. Surfaces
HOBr
HOCl
Dipole Moments
IR Intensities
Calculations

78282. Wang, D., and J.Z.H. Zhang, "Correction of Repulsive Potential Energy Surface for Photodissociation of H_2O in the A-State," *J. Chem. Phys.* 108, 10027-10032 (1998).

P.E. Surface
$H_2O(A)$
Spectra Data
Inversion Method
Repulsive Curves

78283. Kurosawa, T., K. Ohmori, H. Chiba, M. Okunishi, K. Ueda, Y. Sato, A.Z. Devdariani and E.E. Nikitin, "Collision Induced Absorption in Mercury-Rare Gas Collisions," *J. Chem. Phys.* 108, 8101-8109 (1998).

P.E. Curves
HgRg(c,A,B)
Far Wing
(c-X) Absorption
Rg=Ar,Kr,Xe

78284. Merawa, M., and D. Begue, "Dipole Polarizabilities of the Potassium Atom in Its Ground (4^2S) and Excited (4^2P,5^2S) States, and Long-Range Dispersion Interactions between Two K Atoms," *J. Chem. Phys.* 108, 5289-5294 (1998).

P.E. Curves
K_2
Long Range
Dispersion
Interactions
Calculations

78285. Tzeli, D., A. Papakondylis and A. Mavridis, "On the Electronic Structure of NLi_2 and PLi_2, Ground and Low-lying Excited States," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2223-2230 (1998).

P.E. Curves
NLi_2,PLi_2
Low-lying States
Geometries
Binding Energies

78286. Topaler, M.S., D.G. Truhlar, X.Y. Chang, P. Piecuch and J.C. Polanyi, "Potential Energy Surfaces of NaFH," *J. Chem. Phys.* 108, 5349-5377 (1998).

P.E. Surfaces
NaFH
Low-lying States
Na+HF
Reaction Dynamics
Energy Barrier

78287. Smirnov, A.D., "Potential Curves of the Ground Electronic States of Dimers of Sodium, Potassium and Cesium," *Opt. Spectrosc., Russia* 81, 352-357 (1996).

P.E. Curves
Na_2,K_2,Cs_2
Energy Level
Comparisons
Calculation
Method

78288. Petsalakis, I.D., G. Theodorakopoulos, Y. Li, G. Hirsch, R.J. Buenker and M.S. Child, "Theoretical Study on the Rydberg States of NeH: Ab Initio Quantum Defect and Complex Coordinate Calculations," *J. Chem. Phys.* 108, 7607-7615 (1998).

P.E. Curves
NeH,NeD
Rydberg States
Interactions
Predissociations
Lifetimes
Calculations

78289. Cui, Q., and K. Morokuma, "Ab Initio Studies on the Electronic Excited States and Photodissociation of O_3 Anion," *J. Chem. Phys.* 108, 7684-7694 (1998).

P.E. Curves
O_3^-
Low-lying States
Photodissociation
Processes

78290. Tzeli, D., A. Papakondylis and A. Mavridis, "On the Electronic Structure of the Ground ($X^3\Sigma^-$) and Some Low-lying Excited States ($A^3\Pi, a^1\Delta, b^1\Sigma^+, B^3\Sigma^-$) of the Isovalent Species P-Li and P-Na," *J. Mol. Struct.* 417, 277-287 (1997).

P.E. Curves
PLi,PNa
Low-lying States
Spectral Constants
D
Calculations

78291. Alekseyev, A.B., H.-P. Liebermann, R.M. Lingott, O. Bludsky and R.J. Buenker, "The Spectrum of Antimony Hydride: An ab Initio Configuration Interaction Study Employing a Relativistic Effective Core Potential," *J. Chem. Phys.* 108, 7695-7706 (1998).

P.E. Curves
SbH
Low-lying States
Spectral Constants
S/O Splittings
Lifetimes

44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

78292. Yabushita, S., T. Matsushita, U. Nagashima, S. Obara, K. Takano, M. Aoyagi, K. Honda, K. Hashimoto, N. Koba, H. Matsuzawa, S. Yamamoto, S. Yamabe and H. Hosoya, eds., *"Qauntum Chemistry Literature Database: Supplement 16. Bibliography of ab Initio Calculations for 1996," J. Mol. Struct.* 420/421, 743 pp. (1997).

Structural
Calculations
1996 Bibliography
4005 References

78293. Rankin, D.W.H., and H.E. Robertson, "Gas Phase Molecular Structures Determined by Electron Diffraction," *Spectrosc. Properties Inorg. Organometallic Compounds: Chem. Soc. London, Spec. Period Rpt.* 30, 454-470 (1997).

Structures
Electron Diffraction
Inorganics
Organometallics
Review

78294. Parr, R.G., and W. Yang, "Density Functional Theory of the Electronic Structure of Molecules," *Ann. Rev. Phys. Chem.* 46, 701-728 (1995).

Structural
Calculations
DFT Methods
Review

78295. Piechota, J., and M. Suffczynski, "Density Functional Study of the First-Row Transition Metal Monoxides," *Z. Phys. Chem. (Munchen)* 200, 39-49 (1997).

Structural
Calculations
ScO thru CuO
1st Row Transition
Metal Oxides
Spectral Constants
D_0, IPS,EAS

78296. Willis, B.G., and K.F. Jensen, "An Evaluation of Density Functional Theory and ab Initio Predictions for Bridge-Bonded Aluminum Compounds," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2613-2623 (1998).

Structural
Calculations
$Al(CH_3)_2H$
$Al(CH_3)_3$
Dimers,Trimers
Geometries
Frequencies
ΔH_f

78297.	Andrews, L., M. Zhou and W.D. Bare, "Matrix Infrared Spectra and Density Functional Calculations of Three Al, N, O Isomers," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5019-5026 (1998).	Structural Calculations AlON,AlNO NAlO Frequencies Matrix Study Measurements
78298.	Dunning Jr, T.H., and K.A. Peterson, "Use of Moller-Plesset Perturbation Theory in Molecular Calculations: Spectroscopic Constants of First Row Diatomic Molecules," *J. Chem. Phys.* 108, 4761-4771 (1998).	Structural Calculations BH,CH,CO F_2,HF,N_2 Spectral Constants D_e
78299.	Francisco, J.S., and J. Clark, "Study of the Stability of $BrClO_3$ Isomers," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2209-2214 (1998).	Structural Calculations $BrClO_3$ Geometries Frequencies Energies
78300.	Alcami, M., and I.L. Cooper, "Ab Initio Calculations on Bromine Oxide and Dioxides and Their Corresponding Anions," *J. Chem. Phys.* 108, 9414-9424 (1998).	Structural Calculations BrO,BrO_2 BrO^-,BrO_2^- Geometries Frequencies Energies
78301.	Francisco, J.S., "Structure, Vibrational Spectra and Energetics of $OBrO^+$," *Chem. Phys. Lett.* 288, 307-310 (1998).	Structural Calculations BrO_2^+ Geometry Frequencies IP(BrO_2)
78302.	Pasinszki, T., and N.P.C. Westwood, "Unstable Chloronitrile Oxide, ClCNO, and Its Stable Ring Dimer: Generation, Spectroscopy and Structure," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4939-4947 (1998).	Structure CClNO IR Photoelectron Spectra Frequencies Measurements Calculations
78303.	Serrano-Andres, L., N. Forsberg, P.-A. Malmqvist, "Vibronic Structure in Triatomic Molecules: The Hydrocarbon Flame Bands of the Formyl Radical (HCO). A Theoretical Study," *J. Chem. Phys.* 108, 7202-7216 (1998).	Structural Calculations CHO(B,X) CDO(B,X) P.E. Surfaces Frequencies (B-X) Spectral Assignments

78304. Yamaguchi, Y., and H.F. Schaefer III, "An ab Initio Study on the Four Electronically Lowest-lying States of CH_2 Using the State-Averaged Complete Active Space Second-Order Configuration Interaction Method," *Chem. Phys.* 225, 23-31 (1997).

Structural Calculations
CH_2(c,b,a,X)
Frequencies
IR Intensities

78305. Jarzecki, A.A., and E.R. Davidson, "Does Unrestricted Moller-Plesset Perturbation Theory for Low Spin Converge when the System has a Triplet Ground State?," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4742-4746 (1998).

Structural Calculations
CH_2 ,O_2
Triplet States
Unrestricted Method Limitations

78306. Wang, Y., J. Tremmel, J. De Smedt, C. Van Alsenoy, H.J. Geise and B. Van der Veken, "Addition: Ab Initio Determination of the Force Field of Dichloromethane, Verified by Gas Phase Infrared Frequencies and Intensities and Applied to a Combined Electron Diffraction and Microwave Investigation of Geometry [*J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 101, 5919-5925 (1997)]," *ibid.* 102, 3457 (1998).

Structural Calculations
CH_2Cl_2
IR Intensities
Frequencies
Addition

78307. Leszczynski, J., L. Goodman and J.S. Kwiatkowski, "Density Functional Theory and Post-Hartree-Fock Studies on Molecular Structure and Harmonic Vibrational Spectrum of Formaldehyde," *Theor. Chim. Acta* 97, 195-202 (1997).

Structural Calculations
CH_2O
Geometry
Frequencies
IR Spectrum

78308. Del Bene, J.E., S.R. Gwaltney and R.J. Bartlett, "Base Properties of H_2CO in the Excited ($^1n \rightarrow \pi^*$) State," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5124-5127 (1998).

Structural Calculations
CH_2O,CH_3O^+
$CH_2O.HF$
Geometries
Frequencies
Excitation Energies

78309. Stanton, J.F., C.L. Lopreore and J. Gauss, "The Equilibrium Structure and Fundamental Vibrational Frequencies of Dioxirane," *J. Chem. Phys.* 108, 7190-7196 (1998).

Structural Calculations
CH_2OO
Isotopomers
Geometries
Frequencies

78310. Hagen, K., K. Hedberg, E.O. John, R.L. Kirchmeier and J.M. Shreeve, "Structure and Vibrational Force Field of Methyldifluoroamine, CH_3NF_2: An Electron-Diffraction Investigation Augmented by Microwave and Infrared Spectroscopic Data and by ab Initio Molecular Orbital Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5106-5110 (1998).

Structure
CH_3NF_2
Diffraction Study
IR/Microwave
Geometry Measurements
Calculations

78311. Jursic, B.S., "Computation of Geometries and Frequencies of Singlet and Triplet Nitromethane with Density Functional Theory Using Gaussian-Type Orbitals," *Int. J. Quantum Chem.* 64, 263-269 (1997).

Structural Calculations
$^{1,3}CH_3NO_2$
Geometries
Frequencies
^{1,3}Energy Splitting

78312. Jursic, B.S., "Computation of Bond Dissociation Energy for Sulfides and Disulfides with ab Initio and Density Functional Theory Methods," *Int. J. Quantum Chem.* 62, 291-296 (1997).

Structural Calculations
CH_3SH
$(CH_3)_2S$,$(CH_3)_2S_2$
H_2S,H_2S_2
Geometries
D

78313. Bauschlicher Jr, C.W., "The Effect of an Electric Field on the Vibrational Frequency of CN," *Int. J. Quantum Chem.* 61, 859-863 (1997).

Structural Calculations
CN,CN^-
r_e ,ω_e
Dipole Moments
Electric Field Effects

78314. Gutsev, G.L., R.J. Bartlett and R.N. Compton, "Electron Affinities of CO_2 , OCS and CS_2 ," *J. Chem. Phys.* 108, 6756-6762 (1998).

Structural Calculations
CO_2 ,CO_2^-
OCS,OCS^-
CS_2 ,CS_2^-
Geometries
EAs

78315. Sorensen, T.E., and W.B. England, "Valence States of C_2 Feynman's Way," *J. Chem. Phys.* 108, 5205-5215 (1998).

Structural Calculations
C_2
Low-lying States
Spectral Constants
T_e ,D_e

78316. Persson, B.J., P.R. Taylor and J.M.L. Martin, "Ab Initio Calibration Study of the Heat of Formation, Geometry and Anharmonic Force Field of Fluoroacetylene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2483-2492 (1998).

Structural Calculations
FCCH
Geometry
Frequencies
ΔH_f

78317. da Silva, J.B.P., M.N. Ramos and R.E. Bruns, "Effects of Wave Function Modifications on Calculated C-H Vibrational Frequencies and Infrared Intensities of the Dihaloethylenes," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 733-747 (1997).

Structural Calculations
$C_2H_2F_2$
$C_2H_2Cl_2$
Frequencies
IR Intensities
Wave Function Sensitivity

78318. Gutowski, M., K.D. Jordan and P. Skurski, "Electronic Structure of Dipole-Bound Anions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2624-2633 (1998).

Structural Calculations
CH_3CN^-,$C_3H_2^-$
$C_4H_2^-$,$C_5H_2^-$
HCN^-
Anions/Neutrals
Geometries
Frequencies

78319. Nielsen, I.M.B., "Ab Initio Study of Aziridines and Diaziridines: Nitrogen Inversion, Ring Opening and Thermochemistry," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3193-3201 (1998).

Structural Calculations
c-C_2NH_5
c-CN_2H_4
Geometries
Frequencies
CH_3 ,D-Substitution
ΔH_f

78320. Turecek, F., "Proton Affinity of Dimethyl Sulfoxide and Relative Stabilities of C_2H_6OS Molecules and $C_2H_7OS^+$ Ions: A Comparative G2(MP2) ab Initio and Density Functional Theory Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4703-4713 (1998).

Structural Calculations
C_2H_6SO,$C_2H_7SO^+$
Isomers
Geometries
Relative Energies

78321. Cooksy, A.L., "Relocalization in Floppy Free Radicals: Ab Initio Calculations of the C_3H_3O Isomers," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5093-5099 (1998).

Structural Calculations
C_3H_3O
Isomerization Energies
Geometries

78322. Baird, M.S., K. Spencer, S.V. Krasnoshchiokov, Yu.N. Panchenko, N.F. Stepanov and G.R. De Mare, "Ab Initio Vibrational Analysis of Cyclopropene, Its Fluoro Derivatives and Their Deutero Analogues," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2363-2371 (1998).

Structural Calculations
c-C_3H_4
F_1-F_4 ;D_1-D_4
Substitutions
Geometries
Frequencies
Predictions

78323. Thakur, S., V.P. Gupta and B. Ram, "Semiempirical Calculation and Normal Coordinate Study of the Conformation and Electronic and Vibrational Spectra of Acrolein," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 749-759 (1997).

Structural Calculations
CH_2CHCHO
D-Substitution
Geometries
Spectra

78324. Yoshida, H., and H. Matsuura, "Density Functional Study of the Conformations and Vibrations of 1,2-Dimethoxyethane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2691-2699 (1998).

Structural Calculations
$C_2H_4(OCH_3)_2$
Frequencies

78325. Lee, E.P.F., and T.G. Wright, "The Tropyl Cation (c-$C_7H_7^+$) and the Tropyl Radical (c-C_7H_7)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4007-4013 (1998).

Structural Calculations
c-C_7H_7
c-$C_7H_7^+$
Geometries
Frequencies
IP

78326. Valuev, I.A., A.S. Kaklyugin, G.E. Norman and A.V. Pogudin, "Electronic Structure and Bond Energies of Fullerenes C_{60}, C_{70}, C_{76} and C_{78}," *Chem. Phys. Reports* 16, 1069-1078 (1997).

Structural Calculations
C_{60}, C_{70}
C_{76}, C_{78}
Bond Energies

78327. Goodpaster, J.V., J.F. Harrison and V.L. McGuffin, "Ab Initio Study of Polycyclic Aromatic Hydrocarbons in Their Ground and Excited States," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3372-3381 (1998).

Structural Calculations
4 PAHs
Ground/Excited States
Geometries
Frequencies

78328. de Jong, W.A., J. Styszynski, L. Visscher and W.C. Nieuwpoort, "Relativistic and Correlation Effects on Molecular Properties: The Interhalogens ClF, BrF, BrCl, IF, ICl and IBr," *J. Chem. Phys.* 108, 5177-5184 (1998).

Structural Calculations
ClF,BrF,BrCl
IF,ICl,IBr
Spectral Constants
D_e
Relativistic Effects

78329. Janoschek, R., "Bonding Properties of Chlorine Oxides ClO_n(n=1-4) in the Density Functional Theory," *J. Mol. Struct.* 423, 219-224 (1998).

Structural Calculations
ClO,ClO_2
ClO_3,ClO_4
Geometries
Frequencies
D,ΔH_f

78330. Chen, Z., Y. Deng, L. Li and G. Xu, "A Density Functional Theory Study on Stability of Carbonylmetallate Monoanions $Mn(CO)_5^-$, $HFe(CO)_4^-$ and $Co(CO)_4^-$," *J. Mol. Struct.* 417, 247-254 (1997).

Structural Calculations
$Co(CO)_4^-$,$HFe(CO)_4^-$
$Mn(CO)_5^-$
Geometries
Stabilities

78331. Ilias, M., P. Furdik and M. Urban, "Comparative Study of Electron Correlation and Relativistic Effects in CuF, AgF and AuF," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5263-5268 (1998).

Structural Calculations
CuF,AgF,AuF
Spectral Constants
D_e
Dipole Moments

78332. Lee, T.J., C.W. Bauschlicher Jr and D. Jayatilaka, "A Challenge for Density Functional Theory: The XONO and XNO_2 (X=F,Cl and Br) Molecules," *Theor. Chim. Acta* 97, 185-194 (1997).

Structural Calculations
FONO,ClONO
BrONO,FNO_2
$ClNO_2$,$BrNO_2$
Geometries
Frequencies
IR Intensities

78333. Hiberty, P.C., and N. Berthe-Gaujac, "F_4^+: A Stable Three-Electron Bonded Complex and a Challenge for Standard ab Initio Computational Methods," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3169-3174 (1998).

Structural Calculations
F_4^+
Bonding Energies
Geometries

78334. Jang, J.H., J.G. Lee, H. Lee, Y. Xie and H.F. Schaefer III, "Molecular Structures and Vibrational Frequencies of Iron Carbonyls: $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5298-5304 (1998).

Structural Calculations
$Fe(CO)_5$,$Fe_2(CO)_9$
$Fe_3(CO)_{12}$
Geometries
Frequencies

78335. Cao, Z., M. Duran and M. Sola, "Low-lying Electronic States and Molecular Structure of FeO_2 and FeO_2^-," *Chem. Phys. Lett.* 274, 411-421 (1997).

Structural Calculations
FeO_2 ,FeO_2^-
Geometries
Frequencies
Low-lying States
Energies

78336. Maroulis, G., "A Systematic Study of Basis Set, Electron Correlation and Geometry Effects on the Electric Multipole Moments, Polarizability and Hyperpolarizability of HCl," *J. Chem. Phys.* 108, 5432-5448 (1998).

Structural Calculations
HCl
Multipole Moments
Polarizability

78337. Novakovskaya, Yu.V., and N.F. Stepanov, "Structure and Energy of the Positively Ionized Water Clusters," *Int. J. Quantum Chem.* 61, 981-990 (1997).

Structural Calculations
$H_2O_n^+$,n≤4
Geometries
IPS

78338. Tschumper, G.S., and H.F. Schaefer III, "A Comparison between the CISD[TQ] Wave Function and Other Highly Correlated Methods: Molecular Geometry and Harmonic Vibrational Frequencies of MgH_2 ," *J. Chem. Phys.* 108, 7511-7515 (1998).

Structural Calculations
MgH_2
Geometry
Frequencies
6 Methods Compared

78339. Stephens, J.C., Y. Yamaguchi, C.D. Sherrill and H.F. Schaefer III, "X^3B_1, a^1A_1, b^1B_1 and $c^1\Sigma_g^+$ Electronic States of NH_2^+," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3999-4006 (1998).

Structural
Calculations
NH_2^+(c,b,a,X)
Geometries
Frequencies
Energies
IR Intensities

78340. Borisenko, K.B., M. Kolonits, B. Rozsondai and I. Hargittai, "Electron Diffraction Study of the Nitrogen Dioxide Molecular Structure at 294, 480 and 691 K," *J. Mol. Struct.* 413/414, 121-131 (1997).

Structures
NO_2, N_2O_4
Electron
Diffraction
Measurements

78341. Martin, J.M.L., and P.R. Taylor, "Accurate ab Initio Quartic Force Field for *trans*-HNNH and Treatment of Resonance Polyads," *Spectrochim. Acta A. Mol. Spectrosc.* 53, 1039-1050 (1997).

trans-HNNH
Frequencies
Force Field
D-Substitution
Calculations

78342. Ding, F., and L. Zhang, "$HNNH_3$, a New Possible Isomer of N_2H_4: An ab Initio Study," *Int. J. Quantum Chem.* 64, 447-452 (1997).

Structural
Calculations
NH_3NH
Geometry
Frequencies
Isomerization
Energy Barriers

78343. Evangelisti, S., "Ab Initio Study of Nitrogen/Oxygen Clusters: N_2O_3, N_4O_6 and N_8O_{12}," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4925-4929 (1998).

Structural
Calculations
N_2O_3, N_4O_6
N_8O_{12}
Geometries
Frequencies

78344. Zhao, Y., T. Gu, S. Pan and J. Sun, "An ab Initio Study of the Structure, Dissociation Energy and Heat of Formation of Na_2S," *Int. J. Quantum Chem.* 61, 953-957 (1997).

Structural
Calculations
Na_2S
Geometry
Frequencies
D, ΔH_f

78345. Sambrano, J.R., J. Andres, A. Beltran, F. Sensato and E. Longo, "Theoretical Study of the Structure and Stability of Nb_xO_y and $Nb_xO_y^+$ (x=1-3, y=2-5,7,8) Clusters," *Chem. Phys. Lett.* 287, 620-626 (1998).

Structural
Calculations
Nb_xO_y, $Nb_xO_y^+$
Geometries
D, IP

78346. Gan, Z., K. Su, Y. Wang and Z. Wen, "Several Excited States and Thermochemical Properties of PH_n (n=1-3): A High Level ab Initio Study," *Chem. Phys.* 228, 31-38 (1998).

Structural Calculations
PH, PH_2, PH_3
PH^+, PH_2^+, PH_3^+
Geometries
D,IP
Low-lying States

78347. Moussaoui, Y., O. Ouamerali and G.R. De Mare, "Theoretical Study of the Properties of the Radical PS, Its Anion and Cation," *J. Mol. Struct.* 425, 237-247 (1998).

Structural Calculations
PS, PS^+, PS^-
Spectral Constants
D_e,IP,EA

(78397) Structural Calculations, ΔH_f, n=1-6, Geometries, Frequencies — $SF_n, SF_n^{\pm}$

78348. Boldyrev, A.I., J. Simons, J.J. Scherer, J.B. Paul, C.P. Collier and R.J. Saykally, "On the Ground Electronic States of Copper Silicide and Its Ions," *J. Chem. Phys.* 108, 5728-5732 (1998).

Structural Calculations
$SiCu, SiCu^{\pm}$
Low-lying States
Spectral Constants
Energies
D_e,IP,EA

78349. Kishi, R., Y. Negishi, H. Kawamata, S. Iwata, A. Nakajima and K. Kaya, "Geometric and Electronic Structures of Fluorine Bound Silicon Clusters," *J. Chem. Phys.* 108, 8039-8058 (1998).

Structural Calculations
Si_nF, Si_nF^-
Geometries
Energies
n=1-7
EAs

78350. Yamaguchi, Y., T.J. Van Huis, C.D. Sherrill, H.F. Schaefer III, "The X^1A_1, a^3B_1, A^1B_1 and B^1A_1 Electronic States of SiH_2," *Theor. Chim. Acta* 97, 341-349 (1997).

Structural Calculations
SiH_2(B,A,a,X)
Geometries
Energies
IR Intensities

78351. Cai, Z.-L., and J.P. Francois, "Ab Initio Study of the $X^2\Sigma^+$ and $A^2\Pi$ States of the SiO^+ Cation Including the Effect of Core Correlation," *Chem. Phys.* 234, 59-68 (1998).

Structural Calculations
SiO^+(A,X)
Spectral Constants
T_e

78352. Sumathi, R., and M. Hendrickx, "Density Functional and Complete Active Space Self-Consistent Field Investigations on the Structure and Electronic Properties of TiC_n (n=2-4) Clusters," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4883-4889 (1998).

Structural Calculations
TiC_n, n=2-4
Geometries
Isomers
Frequencies
Relative Energies

78353. DiLabio, G.A., and P.A. Christiansen, "Separability of Spin-Orbit and Correlation Energies for the Sixth-Row Main Group Hydride Ground States," *J. Chem. Phys.* 108, 7527-7533 (1998).

Structural Calculations
TlH,PbH,BiH
PoH,AtH
r_e, ω_e, D_e
Spin-Orbit Effects

45. ENERGY TRANSFER

(See also Section 27 for Electronically Excited State Relaxation Processes)

78354. Lim, E.C., "Photophysics of Gaseous Aromatic Molecules: Excess Vibrational Energy Dependence of Radiationless Processes," *Adv. Photochem.* 23, 165-211 (1997).

Electronic/ Vibrational Relaxations
Aromatics
Review

78355. Mo, Y., C. Ottinger, T. Winkler and G. Shen, "Observation of the Electronic Energy Transfer Reaction $CO(a^3\Pi)+NO(X^2\Pi)\rightarrow CO(X^1\Sigma^+)+NO(a^4\Pi)$ in Molecular Beams," *Chem. Phys. Lett.* 274, 451-459 (1997).

E-E Transfer
CO(a) + NO
NO(B,A,a) Channels
Cross Sections

(78182) Unimolecular Dissociation, Slow IVR Nonequilibrations, Generalized Theory

IVR

78356. Doyennette, L., F. Menard-Bourcin, J. Menard, C. Boursier and C. Camy-Peyret, "Vibrational Energy Transfer in Methane Excited to $2\nu_3$ in CH_4-N_2/O_2 Mixtures from Laser Induced Fluorescence Measurements," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3849-3855 (1998).

Vibrational Energy Transfer
$CH_4(2\nu_3)+CH_4$
$CH_4(2\nu_3)+N_2/O_2$
Rate Constants
ν_3, ν_4 Fluorescence Decay Rates

78357. McDowell, D.R., F. Wu and R.B. Weisman, "Vibrational Relaxation of T_1 Pyrazine: Results from the Refined Competitive Radiationless Decay Method," *J. Chem. Phys.* 108, 9404-9413 (1998).

Vibrational Relaxation
c-$C_4H_4N_2(T_1)$
Average Energy Losses
13 Colliders

78358. Wall, M.C., and A.S. Mullin, "'Supercollision' Energy Dependence: State-Resolved Energy Transfer in Collisions between Highly Vibrationally Excited Pyrazine (E_{vib}=37900 and 40900 cm^{-1}) and CO_2," *J. Chem. Phys.* 108, 9658-9667 (1998).

Vibrational Relaxation
c-$C_4H_4N_2(v)+CO_2$
Rate Constants

78359. Wall, M.C., B.A. Stewart and A.S. Mullin, "State-Resolved Collisional Relaxation of Highly Vibrationally Excited Pyridine by CO_2: Influence of a Permanent Dipole Moment," *J. Chem. Phys.* 108, 6185-6196 (1998).

Vibrational Relaxation
c-$C_5H_5N(v)+CO_2$
Rate Constants
CO_2 Product Energies

78360. Mudjijono, and W.D. Lawrance, "State-to-State Vibrationally Excited Transfer in S_1 *p*-Difluorobenzene at Intermediate State Densities: A Change in Propensity Rules," *J. Chem. Phys.* 108, 4877-4886 (1998).

Vibrational Energy Transfer
p-$C_6H_4F_2(S_1)$
Rg,H_2,D_2 Partners
Major Multiquantum
Branching Ratios
Propensities

78361. Heidelbach, C., I.I. Fedchenia, D. Schwarzer and J. Schroeder, "Molecular Dynamics Simulation of Collisional Energy Transfer from Vibrationally Highly Excited Azulene in Compressed CO_2," *J. Chem. Phys.* 108, 10152-10161 (1998).

Vibrational Energy Transfer
$C_{10}H_8(v)+CO_2$
Decay Rates

78362. Ananiev, V.Yu., A.N. Lobanov, A.P. Lytkin and A.V. Khyrbu, "Measuring the Time Constant of Vibrational-Translational Relaxation in Compressed Hydrogen Using Stimulated Raman Scattering," *Bull. Russian Acad. Sci., Phys.* 59, 1013-1020 (1995).

V-T Relaxation
H_2
Rates
Spark Discharge
SRS Monitor

(78125) Vibrational Relaxation Rate Constants

$H_2O(4\nu_{OH})+H$
$H_2O(4\nu_{OH})+H_2O$

78363. Velardez, G.F., R.A. Bollati and J.C. Ferrero, "Quasiclassical Trajectory Simulations of Collisional Vibrationally Excited HgBr($B^2\Sigma$). II. Dependence on Rotational Excitation," *J. Chem. Phys.* 108, 5338-5348 (1998).

Vibrational Relaxation
HgBr(B,v)+Rg
Rotational Energy Effects
Transition Probability Functions

78364. Kozlov, P.V., "Studying Relaxation Processes in a Shock Heated Gas and Ultrasonic Flows Using the CARS Technique," *Bull. Russian Acad. Sci., Phys.* 59, 2121-2125 (1995).

V-T,V-V′ Transfer
N_2,O_2
N_2+N
Shock Tube
CARS Monitor

78365. Akopyan, M.E., N.K. Bibinov and D.B. Kokh, "Vibronic Relaxation of XeF in a Mixture with Inert Gases," *Opt. Spectrosc., Russia* 81, 191-200 (1996).

Vibrational Relaxation
XeF(B,C)+Rg
Channels

78366. Agrawal, P.M., S. Tilwankar and N.K. Dabkara, "The Hard Ellipsoid Potential Model and the Limit of Rotational Energy Transfer in Molecular Collisions," *J. Chem. Phys.* 108, 4854-4861 (1998).

Rotational Energy Transfer
Diatom/Atom
Ellipsoid Potential Model
Validity

46. THERMOCHEMISTRY

78367. Bishnu, P.S., D. Hamiroune, M. Metghalchi and J.C. Keck, "Constrained-Equilibrium Calculations for Chemical Systems Subject to Generalized Linear Constraints Using the NASA and STANJAN Equilibrium Programs," *Combust. Theory Modeling* 1, 295-312 (1997).

Equilibrium Calculations
NASA/STANJAN Code Comparisons

78368. Kafafi, S.A., and E.-S.R.H. El-Gharkawy, "A Simple Coupling Scheme between Hartree-Fock and Local Spin-Density Functional Theories," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3202-3208 (1998).

ΔH_f,IP,EA
New Calculation Method
Accuracies
Computer Times

78369. Fishtik, I., and I. Nagypal, "Thermodynamic Functions: Standard versus Actual Changes in Gas Phase Reactions," *ACH Models in Chemistry* 133, 429-442 (1996).

Thermodynamic Functions
Standard/Actual Changes
Analysis

78370. Bohr, F., and E. Henon, "Comparison of Various Quantum Chemistry Methods for the Computation of Equilibrium Constants," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4857-4862 (1998).

Equilibrium Constants
DFT Methods
Structural Calculations
Accuracies

78371. Mason, R.S., and P.D.J. Anderson, "Comment on the Accuracy of Thermodynamic Data Derived from Studies of Gas Phase Ion-Molecule Equilibria by the Third Law and van't Hoff Methods," *Int. J. Mass Spectrom. Ion Process.* 161, L1-L6 (1997).

Thermodynamic Data
Ion/Molecule Equilibria
Data Accuracy Assessment

(78295) 1st Row Transition Metal Oxides, Structural Calculations, Spectral Constants

D_0,IPS,EAS
ScO thru CuO

(78296) Structural Calculations, Dimers, Trimers, Geometries, Frequencies

$\Delta H_f(Al(CH_3)_2H)$
$\Delta H_f(Al(CH_3)_3)$

78372. Martin, J.M.L., and P.R. Taylor, "Revised Heat of Formation for Gaseous Boron: Basis Set Limit ab Initio Binding Energies of BF_3 and BF," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2995-2998 (1998).

$D_0(BF,BF_3)$
$\Delta H_f(B)$
Calculations

(78298) Structural Calculations, Spectral Constants

$D_e(BH,CH,CO)$
$D_e(F_2,HF,N_2)$

78373. Yu, C.-L., and S.H. Bauer, "Thermochemistry of the Boranes," *J. Phys. Chem. Ref. Data* 27, 807-835 (1998).

Thermochemical Values
26 Boranes
Gas Phase
0-1500 K

(78301) Structural Calculations, Geometry, Frequencies — IP(BrO_2)

78374. Vargas, R., M. Galvan and A. Vela, "Singlet-Triplet Gaps and Spin Potentials," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3134-3140 (1998). — CXY; X,Y=H,F,Cl,Br,I; ^{1,3}Energy Gaps; Vertical/Adiabatic; Calculations

78375. Jarvis, G.K., K.J. Boyle, C.A. Mayhew and R.P. Tuckett, "Threshold Photoelectron-Photoion Coincidence Spectroscopy of Perfluorocarbons. I. Saturated Perfluorocarbons C_2F_6, C_3F_8 and *n*-C_4F_{10}," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3219-3229 (1998). — IP(CF_3); $\Delta H_f(C_3F_7^+)$; Threshold Photoelectron Spectra; C_2F_6,C_3F_8,C_4F_{10}

78376. Litorja, M., and B. Ruscic, "Direct Observation of the Ionization Threshold of Triplet Methylene by Photoionization Mass Spectrometry," *J. Chem. Phys.* 108, 6748-6755 (1998). — IP(CH_2); $\Delta H_f(CH_2(a,X))$; $D_0(CH_3)$; Photoionization Spectral Measurements

78377. Jursic, B.S., "The Density Functional Theory Evaluation of the Heats of Formation of Some Aromatic Compounds Through the Isodesmic Approach," *J. Mol. Struct.* 417, 99-106 (1997). — ΔH_f; CH_2NH,*c*-$C_4H_4N_2$; *c*-C_4H_4O,*c*-C_4H_4S; *c*-C_5H_5N,C_6H_6; DFT/Isodesmic Calculations

(78207) Reaction Enthalpies, Energy Barriers, Calculations — CH_2OH+Alkenes; CH_3+Alkenes; CH_2CN+Alkenes

(78203) Ring Opening/Dissociation Energies, Low-lying States, Reaction Dynamics, CO_2+H_2 Products — *c*-CH_2O_2

(78311) Energy Splitting, Structural Calculations, Geometries, Frequencies — $^{1,3}CH_3NO_2$

(78312) Structural Calculations, Geometries — D; CH_3SH,H_2S,H_2S_2; $(CH_3)_2S$,$(CH_3)_2S_2$

78378. Mayer, P.M., C.J. Parkinson, D.M. Smith and L. Radom, "Erratum - An Assessment of Theoretical Procedures for the Calculation of Reliable Free Radical Thermochemistry: A Recommended New Procedure [*J. Chem. Phys.* 108, 604-615 (1998)]," *ibid.* 9598. — ΔH_f; Free Radicals; New Calculation Procedure; Erratum

78379.	DeTar, D.F., "Theoretical ab Initio Calculation of Entropy, Heat Capacity and Heat Content," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5128-5141 (1998).	Alkanes S, C_p, H_T-H_0 Theoretical Calculation Method
78380.	Chen, C.-J., D. Wong and J.W. Bozzelli, "Standard Chemical Thermodynamic Properties of Multichloro Alkanes and Alkenes: A Modified Group Additivity Scheme," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4551-4558 (1998).	$\Delta H_f, S°, C_p$ Chloroalkanes Chloroalkenes Group Additivity Values
78381.	Lohr, L.L., "Quantum Chemical Studies of Carbon-13 Equilibrium Fractionation in Ion-Molecule Reactions," *J. Chem. Phys.* 108, 8012-8019 (1998).	Reduced Partition Functions CO, HCO^+, HOC^+ Isotopomers $HCO^+, HOC^+/CO$ C^+/CO Exchange Reactions Pathways
78382.	Stimson, S., M. Evans, C.Y. Ng, C.-W. Hsu, P. Heimann, C. Destandau, G. Chambaud and P. Rosmus, "High Resolution Vacuum Ultraviolet Pulsed Field Ionization Photoelectron Band for $OCS^+(X^2\Pi)$: An Experimental and Theoretical Study," *J. Chem. Phys.* 108, 6205-6214 (1998).	IP(OCS) OCS^+ S/O Splitting Vibronic Levels Photoelectron Spectra
(78314)	Structural Calculations, Neutrals/Anions, Geometries	EA(CO_2, OCS) EA(CS_2)
(78315)	Structural Calculations, Low-lying States, Spectral Constants, T_e	$D_e(C_2)$
(78316)	Structural Calculations, Geometry, Frequencies	ΔH_f(FCCH)
(78319)	CH_3- and D-Substitution Effects, Structural Calculations, Geometries, Frequencies`	$\Delta H_f(c\text{-}C_2NH_5)$ $\Delta H_f(c\text{-}CN_2H_4)$
78383.	Knyazev, V.D., "Density of States of One-Dimensional Hindered Internal Rotors and Separability of Rotational Degrees of Freedom," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3916-3922 (1998).	Rotational Partition Functions $i\text{-}C_3H_7, sec\text{-}C_4H_9$ $n\text{-}C_4H_{10}, n\text{-}C_5H_{12}$ Density of States Analytical Formulae
78384.	Ball, D.W., "Density Functional Calculations on the Heats of Formation of Cyclic Hydrocarbons," *J. Mol. Struct.* 417, 107-115 (1997).	ΔH_f Cyclo-alkanes C_3-C_6 Geometries DFT Calculations

78385.	Jarvis, G.K., K.J. Boyle, C.A. Mayhew and R.P. Tuckett, "Threshold Photoelectron-Photoion Coincidence Spectroscopy of Perfluorocarbons. II. Unsaturated and Cyclic Perfluorocarbons C_2F_4, C_3F_6, 2-C_4F_8, and *c*-C_4F_8," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 3230-3237 (1998).	IP(*c*-C_4F_8) $\Delta H_f(C_3F_5^+)$ Threshold Photoelectron Spectra C_2F_4,C_3F_6 2-C_4F_8,*c*-C_4F_8
(78117)	Association Reactions, Thermochemical Estimated Energies, Channels	*c*-C_5H_5/H,O,OH *c*-C_5H_5/HO_2,O_2
(78325)	Structural Calculations, Neutral/Cation, Geometries, Frequencies	IP(*c*-C_7H_7)
78386.	Chen, E.S., E.C.M. Chen and N. Kozanecki, "Comment on the Ionization Potentials and Electron Affinities from the Extended Koopmans' Theorem Applied to Energy Derivative Density Matrices; The EKTMPn and EKTQCISD Methods [*J. Phys. Chem.* 107, 6804-6811 (1997)]," *ibid.* 108, 8749-8750 (1998).	EA Aromatic Hydrocarbons Estimation Method Comment
78387.	Castano, O., R. Notario, R. Gomperts, J.-L.M. Abboud, R. Palmeiro and J.L. Andres, "Heats of Formation of 1,3,5,7-Cyclooctatetraene and Bicyclo[4.2.0]octa-2,4,7-triene: A High Level ab Initio Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4949-4951 (1998).	ΔH_f(*c*-C_8H_8) COT,BOT Calculations
78388.	Rao, Y.K., "An Iterative Computation for Combustion Equilibria," *High Temp. Mater. Sci.* 36, 173-183 (1996).	Equilibrium Calculations JPN Propellant Combustion Method
(78326)	Bond Energies, Structural Calculations	C_{60},C_{70} C_{76},C_{78}
(77948)	Photoassociation Spectrum, r_0'', ω_0'', Measurements	$D_0(Ca^+.C_2H_2)$
(78328)	Structural Calculations, Spectral Constants, Relativistic Effects	D_e(ClF,BrF,BrCl) D_e(IF,ICl,IBr)
(78329)	Structural Calculations, Geometries, Frequencies	D,ΔH_f(ClO,ClO_2) D,ΔH_f(ClO_3,ClO_4)
(77868)	Equilibrium Composition Calculations, Incineration, Gaseous Speciation	Cr
(77801)	$Cr_n^+ + CO_2$ Reactive Cross Sections, n=1-18, Product Ions	$D(Cr_n^+O)$
78389.	Simard, B., M.-A. Lebeault-Dorget, A. Marijnissen and J.J. ter Meulen, "Photoionization Spectroscopy of Dichromium and Dimolybdenum: Ionization Potentials and Bond Energies," *J. Chem. Phys.* 108, 9668-9674 (1998).	IP(Cr_2,Mo_2) D(Cr_2,Mo_2^+) Photoionization Spectra
(77802)	$Cr_n^+ + O_2$ Reactive Cross Sections, n=2-18, Product Ions	$D(Cr_mO_2^+)$

(78331)	Structural Calculations, Spectral Constants, Dipole Moments	D_e(CuF,AgF,AuF)
78390.	Kieninger, M., M. Segovia and O.N. Ventura, "A Discrepancy between Experimental and Theoretical Thermochemical Characterization of Some Oxygen Fluorides," *Chem. Phys. Lett.* 287, 597-600 (1998).	$\Delta H_f(FO,FO_2)$ $\Delta H_f(F_2O,F_2O_2)$ Calculations Recommendations
(78333)	Bonding Energies, Geometries, Structural Calculations	F_4^+
(77952)	R2PI Spectra, Rg=Ar,Kr,Xe, Constants	D_0(GaRg(F,G,H,I,X)
(78105)	CF_3I+OH Rate Constants, Channels	ΔH_f(HOI)
78391.	Peterson, K.A., S.S. Xantheas, D.A. Dixon and T.H. Dunning Jr, "Predicting the Proton Affinities of H_2O and NH_3," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 2449-2454 (1998).	PA(H_2O,NH_3) Calculations
(78337)	n≤4, Geometries, Structural Calculations	IP($H_2O_n^+$)
78392.	Schenter, G.K., "A Quantum Statistical Mechanical Study of the Enthalpy of Formation of the Water Dimer," *J. Chem. Phys.* 108, 6222-6232 (1998).	$\Delta H_f(H_2O)_2$ Calculations
(77962)	(c-X) Pump/Probe Spectrum, Constants	D_0(HgAr(c,X))
(78226)	P.E. Surfaces, H_2NO Systems, Transition State Energies, Calculations	$\Delta H_f(NH_2O)$ ΔH_f(HNOH)
78393.	Trusov, N.V., "Thermodynamic Determination of the Degree of High Temperature Decomposition of Ammonia," *Russ. J. Appl. Chem.* 70, 1190-1193 (1997).	Equilibrium Calculations $NH_3/N_2,H_2$ T,P Dependences
(78285)	Binding Energies, P.E. Curves, Low-lying States, Geometries	NLi_2,PLi_2
78394.	Glukhovtsev, M.N., R.D. Bach and S. Laiter, "High-Level Computational Study on the Thermochemistry of Saturated and Unsaturated Three- and Four-Membered Nitrogen and Phosphorus Rings," *Int. J. Quantum Chem.* 62, 373-384 (1997).	ΔH_f N_3H,P_3H N_3H_3,P_3H_3 N_4H_2,P_4H_2 N_4H_4,P_4H_4 Strain Energies Stabilities
(78344)	Structural Calculations, Geometry, Frequencies	D,$\Delta H_f(Na_2S)$
(78345)	Structural Calculations, Geometries, x=1-3, y=2-5,7,8	D,IP(Nb_xO_y)
78395.	Mazyar, O.A., and T. Baer, "Theoretical and Experimental Studies of Unimolecular Dissociation of Phosphorus Tribromide Ions," *Chem. Phys. Lett.* 288, 327-332 (1998).	$\Delta H_f(PBr_2^+,PBr_3^+)$ IP(PBr_3) Measurements
(78346)	Structural Calculations, Neutrals/Cations, Geometries, Low-lying States	D,IP(PH,PH_2,PH_3)

78396.	Chau, F.-T., J.M. Dyke, E.P.F. Lee, A. Ridha and D.-C. Wang, "He(I) Photoelectron Spectra of PH_2 and PF_2: Comparison between Simulation and Experiment," *Chem. Phys.* 224, 157-173 (1997).	IP(PH_2) IP(PF_2) $^{1,3}PH_2^+$ Splitting $PF_2^+(X,\nu_1)$ $PH_2^+(a,\nu_2)$ Frequencies
(78290)	P.E. Curves, Low-lying States, Spectral Constants, Calculations	D(PLi,PNa)
(78347)	Structural Calculations, Spectral Constants	D_e,IP,EA(PS)
78397.	Bauschlicher Jr, C.W., and A. Ricca, "Accurate Heats of Formation for SF_n, SF_n^+ and SF_n^- for n=1-6," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 4722-4727 (1998).	ΔH_f SF_n,$SF_n^\pm$ n=1-6 Geometries Frequencies Calculations
78398.	Eberhard, J., W.-C. Chen, C.-h. Yu, Y.-P. Lee and B.-M. Cheng, "Photoionization Spectra and Ionization Energies of HSCl, HSSSH, SSCl and HSSCl Formed in the Reaction System $Cl/Cl_2/H_2S$," *J. Chem. Phys.* 108, 6197-6204 (1998).	IPs HSCl,H_2S_3,S_2Cl HS_2Cl,H_2S_2 SCl_2,S_2,S_3 Discharged Cl_2/H_2S Photoionization Spectra
(78245)	Thermochemistries, Gas/Aqueous Phases, Calculations	SO_2+H_2O/H_2SO_3 $SO_2+H_2O/SO_2.H_2O$
(78348)	Structural Calculations, Low-lying States, Spectral Constants, Energies	D_e,IP,EA(SiCu)
78399.	Ricca, A., and C.W. Bauschlicher Jr, "Accurate D_0 Values for SiF and SiF^+," *Chem. Phys. Lett.* 287, 239-242 (1998).	$D_0(SiF,SiF^+)$ Calculations
(78349)	n=1-7, Structural Calculations, Geometries, Energies	EA(Si_nF)
78400.	Hildenbrand, D.L., and K.H. Lau, "Comment on the Thermochemistry of Gaseous SiO(OH), $SiO(OH)_2$ and SiO_2 [*J. Chem. Phys.* 101, 6076-6079 (1994)]," *ibid.* 108, 6535 (1998).	ΔH_f(SiO(OH)) Reassessment
(77993)	n=2-4), Photoelectron Spectra, Frequencies	EA(Si_nH)
(77903)	TiB, TiB_2 Formation, Products, Equilibrium Calculations	$TiCl_4/BCl_3/Na$ $TiCl_4/Na$
(78353)	r_e, ω_e, Spin-Orbit Effects, Structural Calculations	D_e(TlH,PbH,BiH) D_e(PoH,AtH)
(77995)	n=1-4, Photoelectron Spectra, Low-lying States, Constants, Energies	EA(VO_n)
(77813)	n=2-15, $V_n^+ + O_2$ Reactive Channels, n=2-17, Energy Dependences	$D(V_n^+-O)$

78401. Schroder, D., J.N. Harvey, M. Aschi and H. Schwarz, "Experimental and Computational Study of Neutral Xenon Halides (XeX) in the Gas Phase for X=F, Cl, Br and I," *J. Chem. Phys.* 108, 8446-8455 (1998). | Bond Strengths; $XeX, XeX^{\pm}$; X=F,Cl,Br,I; Measurements; Calculations

47. EXPERIMENTAL METHODS

(78054) Photodetectors, Optical Monitoring, Monograph | CCD Arrays

78402. De Goy, S., D. Lanzisera, K. Lopez, J. Noonan and J. Rebello, "Which CCD Detector Is Right for You?," *Spectroscopy* 13(10), 36-42 (1998). | CCD Detectors; UV/Near IR; Performance; Choices

78403. Morland, P., C. Chatillon and P. Rocabois, "High Temperature Mass Spectrometry Using the Knudsen Effusion Cell. I. Optimization of Sampling Constraints on the Molecular Beam," *High Temp. Mater. Sci.* 37, 167-187 (1997). | Knudsen Cell/; Molecular Beam; Mass Analysis; Sampling; Optimization

78404. Lukomskii, N.G., V.A. Polishchuk and M.P. Chaika, "Experimental Observation of Alignment of the $1s_5$ Metastable State of Neon in a Glowing Discharge Plasma," *Opt. Spectrosc., Russia* 81, 333-335 (1996). | Alignment; Degree; $Ne(1s_5)$; Glow Discharge; Measurement

48. MISCELLANEOUS

78405. Trigg, G.L., ed., *"Encyclopedia of Applied Physics,"* Published in 23 Volumes, VCH Publishers, New York (1991-1998). | Applied Physics; Advanced; Encyclopedic; Treatise

78406. Fenn, J.B., "Research in Retrospect: Some Biograffiti of a Journeyman Chemist," *Ann. Rev. Phys. Chem.* 47, 1-41 (1996). | J.B. Fenn; Supersonic Jet; Spectroscopy; Biography

78407. Klemperer, W., "Some Spectroscopic Reminiscences," *Ann. Rev. Phys. Chem.* 46, 1-26 (1995). | W. Klemperer; Spectroscopic; Reminscences

SUBJECT INDEX CATEGORIES

1. Fuels, Synfuels - General
2. Liquefaction, Gasification
3. Burners
4. Coal, Particle Combustion, Pyrolysis
5. Spray Combustion
6. Metals, Propellants, Polymer Combustion
7. Catalytic Combustion
8. MHD
9. Temperatures
10. Ignition
11. Combustion Theory, Propagation, Stabilization
12. Turbulence
13. Detonations, Explosions
14. Flow Phenomena, Velocities, Diffusion
15. Ionization
16. Inhibition, Additives
17. Corrosion, Erosion, Deposition
18. Gas, Surface Interactions, Boundary Layer Combustion
19. Engines, Emissions
20. Plume, Stack Chemistry, Atmospheric Emissions
21. Combustion Emissions, NO_x , SO_2 Chemistry, Control
22. Soot, Diamond, Particle Formation, Control
23. Particle Characterization
24. Nucleation, Coagulation, Clusters
25. Flame, Chemiluminescent Spectroscopy
26. Spectral Characterizations, Analyses
27. Excited State Lifetimes, Quenching
28. Franck-Condon Factors, Transition Probabilities
29. Lineshapes, Strengths
30. Analysis, Monitoring Techniques
31. Flame Concentration Measurements
32. Mapping, Tomographic Methods
33. Optogalvanic, Optoacoustic Methods
34. Flame Kinetic Modeling
35. Pyrolysis Kinetics, Studies
36. Kinetic Modeling, Sensitivities, Rate Constants
37. Photolysis, MPD
38. Reaction Product - Energy Distributions
39. Unimolecular Processes
40. Chemical Dynamics - Theory
41. Chemical Kinetics - General
42. Lasers, Induced Effects, MPI
43. P.E. Curves, Surfaces, Energy Levels
44. Atomic, Molecular Structures
45. Energy Transfer
46. Thermochemistry
47. Experimental Methods
48. Miscellaneous

BIBLIOGRAPHY - JOURNAL COVERAGE

The present master list of journals included in the Bulletin is reproduced here. These issues all are browsed through at first hand to ensure as complete a coverage as possible of all pertinent articles of interest to the many diverse aspects of interest to the combustion scientist and engineer. New journals continue to emerge and are added as they are encountered. Relevant new books and published conferences and symposia also are included. Some of these have been added to this list if they form well-established series. Most of the Russian journals now have modified their titles, eliminating references to Soviet or USSR.

MASTERLIST

ACH Models in Chemistry
Acc. Chem. Res.
Acoust. Soc. Am. J.
ACS Monograph Ser.
ACS Symp. Ser.
Acta Astr.
Acta Chem. Scand., Ser. A
Acta Chim. Hung. (now *ACH Models in Chemistry*)
Acta Chim. Sin. (now *Chinese J. Chem.*)
Acta Phys. Hung.
Acta Phys. Pol. A
Acta Phys. Slovaca
Adv. At. Mol. Phys.
Adv. Atm. Sci.
Adv. Chem. Eng.
Adv. Chem. Phys.
Adv. Chem. Ser.
Adv. Classical Trajectory Methods
Adv. Detailed Reaction Mechanisms
Adv. Electron. Electron Phys.
Adv. Electron. Electron Phys. Suppl.
Adv. Energy Systems Technol.
Adv. Environ. Sci.
Adv. Environ. Sci. Eng.
Adv. Free Radical Chem. (D.D. Tanner, ed.)
Adv. Gas Phase Ion Chem.
Adv. Gas Phase Photochem. Kinet.
Adv. Geophys.
Adv. Heat Transfer
Adv. Infrared Raman Spectrosc. (now *Adv. Spectrosc.*)
Adv. Inorg. Chem.
Adv. Laser Spectrosc. (B.A. Garetz, ed.)
Adv. Mass Spectrom.
Adv. Mol. Electron. Structure Theory
Adv. Mol. Relax. Process. (now *J. Mol. Liquids*)
Adv. Molecular Modeling
Adv. Molecular Vibrations Collision Dynam.
Adv. Multiphoton Process. Spectrosc.
Adv. Photochem.
Adv. Phys.
Adv. Quantum Chem.
Adv. Quantum Electron. (ceased publ.)
Adv. Ser. Fullerenes
Adv. Ser. Phys. Chem.
Adv. Space Res. (COSPAR)
Adv. Spectrosc.
Adv. Thermophys. Ser.
Advanced Mater.
Aerosol Sci. Technol.
Aerospace America
AIAA J.
AIAA Papers
AIChE J.
AIChE Symp. Ser.
AIChE Monograph Ser.
Air Pollut. Control Assoc. J. (changed to *J. Air Waste Manage. Assoc.*)
Air & Waste (now *J. Air WasteManage. Assoc.*)
Alternate Energy Sources, Miami Int. Conf.
Am. Inst. Phys. Conf. Proc.
Am. J. Phys.
Anales Fis.
Anal. Chem.
Anal. Chim. Acta
Anal. Commun.
Anal. Lett.
Anal. Proc. (now *Anal. Commun.*)
Anal. Sci. Jpn.
Analyst
Angew. Chem. Int. Ed. Engl.
Angew Chem. Suppl. (ceased publ.)
Ann. de Phys.
Ann. de Phys. Colloq.
Ann. Geophys.
Ann. N.Y. Acad. Sci.
Ann. Phys. N.Y.
Ann. Physik
Ann. Rpts. Anal. At. Spectrosc.
Ann. Repts. Prog. Chem. A. Inorg. Chem.
Ann. Repts. Prog. Chem. C Phys. Chem.
Ann. Rev. Astron. Astrophys.
Ann. Rev. Earth Planet. Sci.

Ann. Rev. Energy Environ.
Ann. Rev. Fluid Mech.
Ann. Rev. Numerical Fluid Mech.
Ann. Rev. Phys. Chem.
Ann. Soc. Sci. Bruxelles (ceased publ.)
Appl. Energy
Appl. Energy: Russian J. Fuel, Power, Heat Systems (previously *Power Engineering, Russ. Acad. Sci.*)
Appl. Opt.
Appl. Phys. B. Lasers Opt.
Appl. Phys. Commun.
Appl. Phys. Lett.
Appl. Sci. Res.
Appl. Spectrosc.
Appl. Spectrosc. Rev.
Appl. Thermal Eng.
Appl. Thermal Sci.
Archivum Combustionis
Astron. Astrophys.
Astron. Astrophys. Rev.
Astron. Astrophys., Suppl. Ser.
Astronaut. Aeronaut (now *Aerospace Am.*)
Astrophys. J.
Astrophys. J. Suppl. Ser.
Astrophys. Lett.
Astrophys. Space Sci.
Astrophys.,Russia
At. Data Nucl. Data Tables
At. Phys.
At. Spectrosc.
Atm. Environ.
Atm. Ocean Phys. Izv. Russian Acad. Sci. (see *Izv. Ocean. Phys.*)
Atm. Ocean
Atm. Optics, Russia
Atm. Research(formerly *J. de Recherches Atmospheriques*)
Atomization Spray Technol. (merged into *Aerosol. Sci. Technol.*)
Atomization Sprays
Aust. J. Chem.
Aust. J. Phys.
Auto. Eng.
Beitrage Plasmaphys. (now *Contributions to Plasmaphys.*)
Ber. Bunsenges. Phys. Chem.
Brazilian J. Phys. (formerly *Rev. Brasil. Fis.*)
Bull. Acad. Sci. USSR, Chem. Sci. (now *Russian Chem. Bull.*)
Bull. Acad. Sci. USSR, Phys. Ser. (now *Bull. Russian Acad. Sci. Phys.*)
Bull. Am. Phys. Soc.
Bull. Chem. Soc. Jpn .
Bull. Classe Sci. Acad. Royal Belg.
Bull. Lebedev Phys. Inst. (formerly *Sov. Phys. Lebedev Inst. Rpts.*)
Bull. Polish Acad. Sci. Chem.
Bull. Russian Acad. Sci., Phys (formerly *Bull. Acad. Sci. USSR, Phys. Ser.*)
Bull. Soc. Chim. Belg.
Bull. Soc. Chim. Fr.
Bull Soc. Mech. Eng. Jpn. (now *JSME Int. J.*)
C1 Molecule Chem.
Calphad: Comput. Coupling Phase Diag. Thermochem.
Can. Aeronaut. Space J.
Can. J. Anal. Sci. Spectrosc.
Can. J. Appl. Spectrosc. (now *Can. J. Anal. Sci. Spectrosc.*)
Can. J. Chem.
Can. J. Chem. Eng.
Can. J. Phys.
Can. J. Spectrosc. (now *Can. J.Anal. Sci. Spectrosc.*)
Carbon
Catalysis, Chem. Soc. Lond., Spec. Period. Rpt.
Chaos
Chem. Berichte
Chem. Bio. Appl. Lasers (C.B. Moore, ed.)
Chem. Britain
Chem. Commun.
Chem. Eng. Commun.
Chem. Eng. J.
Chem. Eng. News
Chem. Eng. Res. Design. Trans. Inst. Chem. Eng.
Chem. Eng. Sci.
Chem. Eur. J.
Chem.Express: J. Kinki Chem. Soc. Jpn.
Chem. Lett. Jpn.
Chem. Materials
Chem. Papers Slovak Acad. Sci. (*Chemicke Zvesti*)
Chem. Phys.
Chem. Phys. Lett.
Chem. Phys. Reports Russia (formerly *Soviet J. Chem. Phys.*)
Chem. Rev.
Chem. Scr. (ceased publ.)
Chem. Soc. (Lond.) Spec. Publ.
Chem. Soc. Rev.
Chem. Technik
Chem. Technol. Fuels Oils, Russia

Chem. Technol. Rev. (Noyes Data)
Chem. Thermodyn. Chem. Soc. Land., Spec. Period Rpt.) (ceased publ.)
Chem. Vap. Deposition
Chemicke Listy, Rocnik
Chemicke Zvesti (Chem. Papers Slovak Acad. Sci.)
Chemiker Zeitung (now merged with *J. Prak. Chem.*)
Chemosphere
Chimica Chronika
Chinese J. Chem. (formerly *Acta Chim. Sin.*)
Chinese J. Eng. Thermophys.
Chinese Phys. (ceased publ.)
Chinese Phys. Lasers (ceased publ.)
Chinese Phys. Lett.
Chinese Sci. Bull.
CLEO Conf. Lasers Electro-opt. Proc.
Climate Dyn.
Climatic Change
Coal Science (M.L. Gorbaty et al., eds.)
Coal Sci. Technol.
CODATA Bull.
CODATA Newslett.
Coke & Chem., Russia
Collect. Czech. Chem. Commun.
Combust. Expl. Shock Waves, Russia
Combust. Flame
Combust. Sci. Technol.
Combust. Theory Modeling
Comments At. Mol. Phys.
Comments Inorg. Chem.
Commun. Appl. Numer. Methods. (now *Commun. Numer. Methods Eng.*)
Commun. Numer. Methods Eng. (formerly *Commun. Appl. Numer. Methods*)
Comp. Chem. Kinet.
Compt. Rendus Acad. Sci., Paris, Ser. II, Part a. Earth Planet. Sciences
Compt. Rendus Acad. Sci.., Paris, Ser. II Part b. Mecanique, Physique, Chemie, Astronomie
Comput. Chem. Eng.
Comput. Phys. Commun.
Computers & Chem.
Computers & Fluids
Computers in Phys.
Contemp. Phys.
Contrib. Atmos. Phys.
Contrib. Plasma Phys.
Corrosion
Corrosion Sci.
Crit. Rev. Anal. Chem.
Crit. Rev. Environ. Control (now *Crit.Rev. Environ. Sci. Technol.*)
Crit. Rev. Environ. Sci. Technol. (formerly *Crit. Rev. Environ. Control*)
Curr. Sci. India
Czech. J. Phys.
DLR Nachrichten
Diamond Related Mater.
Dokl. Chem.
Dokl. Phys. Chem.
Dyn. Atm. Oceans
Earth Plant. Sci. Lett.
Electro-Optic Systems J. (now *Laser Focus*)
Endeavor
Energy
Energy Biomass Wastes
Energy Environ.
Energy Fuels
Energy Research
Energy Sources
Energy Technol. Rev. (Noyes Data)
Environ. Chem., Chem. Soc. London., Spec. Period Rpt.
Environ. Progress
Environ. Sci. Technol.
Environ. Technol.
Environ. Technol. Lett. (now *Environ. Technol.*)
EPRI J.
EPRI Reports
Essays Chem. (ceased publ.)
Eur. J. Phys.
Eur. Turbulence Conf. Adv. Turbulence
Europhys. Lett.
Excited States (E.C. Lim, ed.)
Exp. Technik Phys.
Experimental Heat Transfer
Experimental Thermal Fluid Sci.
Experiments Fluids
Faraday Discuss. Chem. Soc.
Faraday Symp. Chem. Soc. (merged with *J. Chem. Soc. Faraday Trans.*)
Finnish Chem. Lett. (ceased publ.)
Fire Materials
Fire Safety J.
Fire Technol.
Flame Retard. Polym. Mat. (M. Lewin et al., eds.)
Flow Measurement Instrumentation
Fluid Dyn. Res.
Fluid Dyn., Russia

Fluid Mech. Res. (formerly *Fluid Mech. Sov. Res.*)
Fluid Mech. Sov. Res. (now *Fluid Mech. Res.*)
Fluidization, Eng. Foundation Conf.
Fluorine Chem. Rev. (ceased publication)
Fluorocarbons, Chem. Soc. Lond., Spec. Period. Rpt. (ceased publ.)
Fly Ash Coal Conversion Symp.
Fuel
Fuel Sci. Technol. Int.
Fullerene Sci. Technol.
GAMM Conf. Numer. Methods Fluid Mech.
Gazz. Chim. Ital.
Geomagn. Aeron., Russia
Geophys. Monographs
Geophys. Res. Lett.
Global Atmosphere Ocean System
Handbook Environ. Chem.
Hazardous Waste Hazard. Mater.
Heat Mass Transfer (previously *Warme und Stoffubertragung*)
Heat Technol.
Heat Transfer Fluid Mech. Inst. Proc.
Heat Transfer Jpn. Res.
Heat Transfer Res. (formerly *Heat Transfer Sov. Res.*)
Heat Transfer Sov. Res. (now *Heat Transfer Res.*)
Helv. Chim. Acta
Helv. Phys. Acta
High Energy Chem., Russia
High Purity Substances, Russia
High Temp. Mater. Process.
High Temp. Mater. Sci.
High Temp. Technol (now *Mater. High Temp.*)
High Temp., Russia
Hydrogen Energy Progress, Proc. World Conf.
Icarus
I.Ch.E. Symp. Ser.
IEE Proc. J. Optoelectron.
IEEE J. Quantum Electron.
IEEE J. Selected Topics Quantum Electron.
IEEE Trans. Plasma Sci.
I.Mech.E. Conf. Publ.
Ind. Eng. Chem. Fundament. (now *Ind. Eng. Chem. Res.*)
Ind. Eng. Chem. Process Design Develop. (now *Ind. Eng. Chem. Res.*)
Ind. Eng. Chem. Product Res. Develop. (now *Ind. Eng. Chem Res.*)
Ind. Eng. Chem. Res (merging of *Ind.Eng. Chem. Fundament., Process Design Develop., Product Res. Develop.*)
Ind. Res. Develop. (now *Res. Develop.*)
Indian J. Chem. A
Indian J. Phys. B
Indian J. Pure Appl. Phys.
Indian J. Radio Space Phys.
Indian J. Technol.
Infrared Phys. Technol.
Inorg. Chim. Acta
Inorganic Chem.
Int. Commun. Heat Mass Transfer
Int. Conf. Coal Sci.
Int. Conf. Fluidized Bed Combust.
Int. Conf. Laser Spectrosc.
Int. Conf. Multiphase Flow
Int. Conf. Numer. Methods Fluid Dyn.
Int. Conf. Numer. Methods Laminar Flow
Int. Conf. Phys. Electron. At. Collisions
Int. Conf. Spectral Lineshapes
Int. Heat Transfer Conf.
Int. J. Bifurcation Chaos
Int. J. Chem. Kinet.
Int. J. Energy Res.
Int. J. Eng. Fluid Mech.
Int. J. Eng. Sci.
Int. J. Environ. Anal. Chem.
Int. J. Global Energy Issues
Int. J. Heat Fluid Flow
Int. J. Heat Mass Transfer
Int. J. Hydrogen Energy
Int. J. Mass Spectrom. Ion Process.
Int. J. Multiphase Flow
Int. J. Numer. Methods Eng.
Int. J. Numer. Methods Fluids
Int. J. Optoelectronics
Int. J. Quantum Chem.
Int. J. Quantum Chem. Symp.
Int. J. Refractory Hard Metals
Int. J. Thermophys.
Int. J. Turbo Jet Eng.
Int. Meeting Optogalvanic Spectrosc.
Int. Quantum Electron. Conf.
Int. Rev. Phys. Chem.
Int. Ser. Monographs Chem.
Int. Ser. Monographs Phys.
Int. Symp. Flow Visualization
Int. Symp. Gaseous Dielectrics
Int. Symp. Plasma Chem.
Int. Symp. Rarefied Gas Dyn.
Int. Symp. Resonance Ioniz. Spectrosc.

Int. Symp. Turbulent Shear Flows
Intersoc. Energy Conv. Eng. Conf. Proc.
Isr. J. Chem.
Isr. J. Technol.
Izv. Atm. Ocean. Phys.
J. Aerosol Sci.
J. Aerospace Eng., Proc. Inst. Mech. Eng. G.
J. Air Waste Manage. Assoc.
J. Aircraft
J. Alloys Compounds
J. Am. Chem. Soc.
J. Am. Soc. Mass Spectrom.
J. Anal. Appl. Pyrolysis
J. Anal. At. Spectrom.
J. Anal. Chem., Russia
J. Appl. Chem., Russia (now *Russian J. Appl. Chem.*)
J. Appl. Mech. Techn. Phys., Russia
J. Appl. Mech., Trans. ASME
J. Appl. Meteor (now *J. Climate Appl. Meteor*.)
J. Appl. Phys.
J. Appl. Spectrosc., Russia
J. Astrophys. Astron.
J. Atm. Chem.
J. Atm. Ocean Technol.
J. Atmos. Sci.
J. Atmos. Solar-Terr. Phys.
J. Auto. Eng., Proc. Inst. Mech. Eng. D.
J. Biolum. Chemilumin.
J. Chem. Educ.
J. Chem. Eng. Data
J. Chem. Eng. Japan
J. Chem. Phys.
J. Chem. Res.
J. Chem. Soc., Chem. Commun. (now *Chem. Commun.*)
J. Chem. Soc., Dalton Trans.
J. Chem. Soc., Faraday Trans.
J. Chem. Soc. Pakistan
J. Chem. Soc., Perkin Trans., I. Org. Bio-org. Chem.
J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.
J. Chem. Thermodyn.
J. Chinese Chem. Soc.
J. Chinese Inst. Chem. Eng.
J. Chromat. Sci.
J. Climate
J. Climate Appl. Meteor.
J. Cluster Sci.
J. Computat. Chem.
J. Computat. Phys.
J. de Chim. Phys.
J. de Phys. I. General Phys.
J. de Phys. II. Chem. Phys.
J. de Phys. III. Master Sci.
J. de Phys. IV. Colloque
J. de Phys. Colloq. (now *J. de Phys. IV)*
J. de Phys. Lett. (now *Europhys. Lett.*)
J. Electrochem. Soc.
J. Electron Spectrosc. Relat. Phenom.
J. Energy (ceased publ.)
J. Energy Resources Technol., Trans. ASME
J. Eng. Phys. Thermophys., Russia
J. Eng. Gas Turb. Power, Trans. ASME
J. Enhanced Heat Transfer
J. Exp. Theoret. Phys. (formerly *Sov.Phys., JETP*)
JETP Lett.
J. Fire Sci.
J. Fluid Mech.
J. Fluids Eng., Trans. ASME
J. Fluids Structures
J. Fluorine Chem.
J. Gen. Chem. USSR (now *Russ. J. Gen. Chem.*)
J. Geophys. Res.
J. Hazardous Mat.
J. Heat Transfer, Trans ASME
J. Imaging Sci.
J. Indian Chem. Soc.
J. Indian Inst. Sci.
J. Inst. Energy
J. Korean Phys. Soc.
J. Less-Common Met. (now *J. Alloys Compounds*)
J. Mass Spectrom.
J. Mater. Chem.
J. Mater. Res.
J. Mater. Sci.
J. Mater. Sci. Lett.
J. Math. Chem.
J. Mech. Eng. Sci., Proc. Inst. Mech. Eng. C.
J. Microsc. Spectrosc. Electron. (continued as *Microsc. Microanal. Microstruct.*)
J. Modern Opt.
J. Mol. Graphics
J. Mol. Liquids
J. Mol. Spectrosc.
J. Mol. Struct.
J. Nuclear Materials

J. Opt. Soc. Am. A. Optics, Image Sci., Vision
J. Opt. Soc. Am. B. Opt. Phys.
J. Opt. Technol. (formerly *Sov. J. Opt. Technol.*)
J. Optics (Paris)
J. Photoacoust. (ceased publ.)
J. Photochem. Photobiol. A. Chem.
J. Phys. A:. Mathematical General
J. Phys. B At. Mol. Opt. Phys.
J. Phys. D: Appl. Phys.
J. Phys. E (now *Measurement Sci. Technol.*)
J. Phys. Chem. A. Mol., Spectrosc., Kinetics
J. Phys. Chem. B. Mater., Surfaces, Interfaces
J. Phys. Chem. Ref. Data
J. Phys. Chem. Solids
J. Phys. Soc. Jpn. (see *Phys. Soc. Jpn. J.*)
J. Power Energy, Proc. Inst. Mech. Eng. A.
J. Prakt. Chem.
J. Propulsion Power
J. Quant. Spectrosc. Radiat. Transfer
J. Raman Spectrosc.
J. Res. Natl. Inst. Stand. Technol.
J. Russian Laser Res.
J. Sov. Laser Res. (now *J. Russ. Laser Res.*)
J. Spacecraft Rockets
J. Struct. Chem., Russia
J. Thermal Anal.
J. Thermophys. Heat Transfer
J. Turbomach., Trans. ASME
Jpn. J. Appl. Phys.
Jpn. J. Appl. Phys. Lett. A,B
JSAE Review
JSME Int. J. Ser. B. Fluids Thermal Eng. (formerly *JSME Int. J. Ser. II*)
JSME Int. J. Ser. II (formerly *Bull. JSME*, now *JSME Int. J. Ser. B. Fluids Thermal Eng.*)
Kinet. Catal., Russia
Lanthanide Actinide Res. (ceased publ.)
La Recherche Aerospatiale (Eng. Ed.)
Laser Applications
Laser Chem.
Laser Focus World
Laser Interaction (H.J. Schwartz et al., eds.)
Laser Opto-Electron. Conf. Proc.
Laser Optronics (formerly *Lasers Applic.*)
Laser Phys., Russia
Lasers (Proc. Int. Conf., STS Press, McLean VA)
Lasers and Applications (now *Laser Optron.*)
Lect. Notes Chem.
Lect. Notes Phys.
Lect. Notes Phys. New Ser. Monographs
Lett. Nuovo Cimento (now *Europhys. Lett.*)
Lithuanian Phys. J.
Magnetohydrodynamics
Magnetohydrodyn., Russia
Mass Spectrom., Chem. Soc. Lond., Spec. Period. Rpt.
Mass Spectrom. Rev.
Mater. Chem. Phys.
Mater. High Temp.
Mater. Lett.
Mater. Res. Bull.
Materials Research Soc. Symp. Proc.
Measurement Sci. Technol.
Mech. Eng.
Mem. Natl. Def. Acad. Jpn.
Mem. Fac. Sci. Kyushu Univ. Jpn. C. Chem.
Mendeleev Chem. J.
Mendeleev Commun.
Microchem. J.
Microsc. Microanal. Microstruct.
Mod. Fluoresc. Spectrosc. (E.L. Webry, ed.)
Mol. Interactions (H. Ratajczak et al., eds.)
Mol. Photochem. (ceased publ.)
Mol. Phys.
Mol. Spectrosc., Chem. Soc. Lond., Spec. Period. Rpt. (ceased publ.)
Mol. Struct. Energetics
Mon. Not. Roy. Astron. Soc.
Monogr. Mod. Chem.
Moscow Univ. Chem. Bull.
Moscow Univ. Phys. Bull.
NATO Adv. Study Instit. Ser. B. Phys.
NATO Adv. Study Instit. Ser. C. Math. Phys. Sci.
NATO Adv. Study Instit. Ser. E. Appl. Sci.
NATO Adv. Study Instit. Ser. I. Global Environ. Change
NATO Conf. Ser. II. Systems Sci.
NATO Conf. Ser. VI. Mater. Sci.
Nature
Naturwissenschaften
New J. Chem.
New Publ. Bur. Mines
Nonlinearity
Notes Numer. Fluid Mech.
Numer. Heat Transfer A. Applications
Numer. Heat Transfer B. Fundamentals
Numer. Methods Non-linear Problems
Numer. Methods Thermal Problems
Nuov. J. Chem. (now *New J. Chem.*)
Nuovo Cimento B: General Phys.
Nuovo Cimento C: Geophys. Space Phys.

Nuovo Cimento D: Condensed Matter, At. Mol. Chem. Phys.
Opt. Commun.
Opt. Eng.
Opt. Laser Technol.
Opt. Lasers Eng. Int. J.
Opt. Lett.
Opt. Pura Appl.
Opt. Quantum Electron.
Opt. Soc. Am. Proc.
Opt. Spectrosc., Russia
Optica Acta (now *J. Modern Opt.*)
Oxidation Commun.
Oxidation Metals
Ozone Sci. Eng.
PAH Symp. Proc.
Particle Part. Syst. Charact.
Particle Size Anal. Conf.
Particulate Sci. Technol.
Phenomena Ionized Gases
Photochem., Chem. Soc. Lond., Spec. Period. Rpt.
Phil. Trans. Roy. Soc. Lond. A
Philips J. Res.
Philips J. Res., Suppl.
Phosphorus Sulfur
Photochem. Photobiol.
Photonics Spectra
Phys. Doklady (formerly *Sov. Phys. Doklady*)
Phys. Fluids (formerly *Phys. Fluids A*)
Phys. Fluids A,B (now *Phys. Fluids* and *Phys. Plasmas*)
Phys. Lett. A
Phys. Plasmas (formerly *Phys. Fluids B*)
Phys. Quantum Electron.
Phys. Rev. A: At. Mol. Opt. Phys.
Phys. Rev. E: Statist. Phys., Plasmas, Fluids
Phys. Rev. Lett.
Phys. Scr.
Phys. Scr. Colloq.
Phys. Soc. Jpn. J.
Phys. Technol. (now *Phys. World*)
Phys. Today
Phys. Usp., Russia (formerly *Sov. Phys. Usp.*)
Phys. World
Physica (Amsterdam) A. Statist. Theor. Phys.
Physica (Amsterdam) D. Nonlinear Phenom.
PhysicoChem. Hydrodyn (absorbed into *Int. J. Multiphase Flow*)
Planet. Space Sci.
Plasma Chem. Plasma Process.
Polish J. Chem. (transl. of *Rocz. Chem.*)
Pollut. Technol. Rev. (Noyes Data)
Power Eng., Russ. Acad. Sci. (now *Appl. Energy: Russian J. Fuel, Power, Heat Systems*)
Pramana J. Phys. (India)
Proc. Indian Acad. Sci., Chem. Sci.
Proc. Indian Acad. Sci., Earth Planet Sci.
Proc. Indian Natl. Sci. Acad. A (New Delhi)
Proc. Inst. Mech. Eng. A. J. Power Energy
Proc. Inst. Mech. Eng. B. J. Mech. Eng. Sci.
Proc. Inst. Mech. Eng. C. J. Auto. Eng.
Proc. Inst. Mech. Eng. G. J. Aerospace Eng.
Proc. Int. Conf. Lasers
Proc. Natl. Acad. Sci. India A
Proc. Nat. Acad. Sci. USA
Proc. Natl. Sci. Council, Taiwan, A. Phys. Sci. Eng.
Proc. Raman Conf.
Proc. Roy. Soc. Lond. A
Proc. (Trudy) Lebedev Phys. Inst.
Prog. Aerospace Sci.
Prog. Anal. At. Spectrosc. (now *Spectrochim. Acta Rev.*)
Prog. Astro. Aeronaut.
Prog. Energy Combust. Sci.
Prog. Inorg. Chem.
Prog. Opt.
Prog. Phys. (now *Rpts. Prog. Phys.*)
Progress Phys. (Series)
Prog. Quantum Electron.
Prog. React. Kinet.
Propellants Expl. Pyrotech.
Property Data Update USSR (ceased publ.)
Publications Math. Research Center, Univ. Wisconsin
Pure Appl. Chem.
Pure Appl. Geophys.
Quantum Electron. USSR (formerly *Sov. J. Quantum Electron.*, now *Russ. J. Quantum Electron.*)
Quantum Opt.
Quantum Theory Chem. React. (R. Daudel et al., eds.), (ceased publ.)
Radiat. Phys. Chem.
Radiat. Res.
Radio Sci.
Radiochem., Chem. Soc. Lond., Spec. Period Rpt. (ceased publ.)
Radiochem, Russia
Radiophys. Quantum Electron. USSR
Rapid Commun. Mass Spectrom.
React. Kinet. Catal. Lett.

React. Kinet., Chem. Soc. Lond., Spec. Period. Rpt.
Reactive Intermediates (R.A. Abramovitch, ed.)
Recl. Trav. Chim. Pays-Bas (absorbed into *Chem. Berichte*)
Remote Sensing Environ.
Research Chem. Intermed (formerly *Reviews Chem. Intermed.*)
Research Chemical Kinetics
Res. Develop.
Rev. Anal. Chem.
Rev. Computat. Chem.
Rev. Geophys. Space Phys.
Rev. Inorg. Chem.
Rev. Inst. Fr. Petrole
Rev. Int. Hautes Temp. Refract.
Rev. Mod. Phys.
Rev. Phys. Chem. Jpn. (ceased publ.)
Rev. Roum. Chim.
Rev. Roum. Phys. (now *Romanian J. Phys.*)
Rev. Sci. Instrum.
Revista Brasil. Fis. (now *Brazilian J. Phys.*)
Romanian J. Phys. (formerly *Rev. Rouman. Phys.*)
Rpts. Inst. Fluid Sci. Jpn.
Rpts. Prog. Phys.
Russ. Aeronaut.(formerly *Sov. Aeronaut.*)
Russ. Chem. Bull. (formerly *Bull. Acad. Sci. USSR*, *Chem. Sci.*)
Russ. Chem. Rev.
Russ. J. Appl. Chem. (formerly *J. Appl. Chem. USSR*)
Russ. J. Gen. Chem. (formerly *J. Gen. Chem. USSR*)
Russ. J. Inorg. Chem.
Russ. J. Phys. Chem.
Russ. J. Quantum Electron. (formerly *Sov. J. Quantum Electron.*)
Russ. Phys. J. (formerly *Sov. Phys. J.*)
SAE Transactions
Selected Ann. Rev. Anal. Sci. (ceased publ.)
Science
Science China A.. Math Phys. Astron.
Science China B. Chem.
Sci. Inform. Bull. ONRFE (ceased publ.)
Sci. Light
Sci. Prog.
Scientia Sinica A,B (see *Science China*)
Scientific Am.
Shock Tube Shock Wave Res., Proc. Int. Symp.
Shock Waves
SIAM J. Appl. Math.
Soc. Photo-Opt. Instrum. Eng. (SPIE) Proc.
Solid Fuel Chem. USSR
South African J. Chem.
South African J. Phys.
Sov. Aeronaut. (now *Russ. Aeronaut.*)
Sov. J. Appl. Phys.
Sov. J. Chem. Phys. (now *Chem. Phys. Reports*)
Sov. J. Opt. Technol. (now *J. Opt. Technol*.)
Sov. J. Quantum Electron. (now *Russ. J. Quantum Electron.*)
Sov. Phys. Collect. (now *Lithuanian Phys. J.*)
Sov. Phys. Dokl. (now *Phys. Doklady*)
Sov. Phys. J. (now *Russ. Phys. J.*)
Sov. Phys. JETP (now *J. Exp. Theoret. Phys.*)
Sov. Phys. Lebedev Inst. Rep. (now *Bull. Lebedev Phys. Inst.*)
Sov. Phys. Techn. Phys. (now *Technical Phys., Russia*)
Sov. Phys. Usp. (now *Phys. Usp., Russia*)
Sov. Prog. Chem. (now *Ukranian Chem. J.*)
Soviet Radiochem. (now *Radiochem.*)
Sov. Sci. Rev. A. Phys.
Sov. Sci. Rev. B. Chem.
Sov. Sci. Rev. C. Math Phys.
Sov. Sci. Rev E. Astrophys. Space Phys.
Sov. Tech. Phys. Lett. (now *Technical Phys. Lett. Russia*)
Space Res. (now *Adv. Space Res.*)
Space Sci. Rev.
Spectrochim. Acta A. Mol. Spectrosc.
Spectrochim Acta B. At. Spectrosc.
Spectrochim. Acta Rev. (absorbed into *Spectrochim. Acta B*)
Spectrosc. Lett.
Spectrosc. Properties Inorg. Organometallic Compounds: Spec. Period. Rpt.
Spectroscopy
Springer Proc. Phys.
Springer Ser. Atoms Plasmas
Springer Ser. Chem. Phys.
Springer Ser. Opt. Sci.
Statist. Mech., Chem. Soc., Lond., Spec. Period. Rpt. (ceased publ.)
Staub Reinhalt Luft
Structural Chem.
Structure Bonding
Studies in Phys. Theoret. Chem.
Sulfur Lett.
Sulfur Reports
Surface Chem.
Survey Prog. Chem. (ceased publ.)
Surveys Geophys.

Symp. (Int.) Combust. Proc.
Talanta
Technical Phys., Russia (formerly *Sov. Phys. Techn. Phys.*)
Technical Phys. Lett., Russia (formerly *Sov. Technical Phys. Lett.*)
Tellus A. Dyn. Meteor. Ocean.
Tellus B. Chem. Phys. Meteor.
Theor. Chem. (Adv. Perspectives), (ceased publ.)
Theor. Chem., Chem. Soc. Lond., Spec. Period, Rpt. (ceased publ.)
Theor. Chim. Acta
Theor. Comput. Fluid Dynam.
Theor. Exp. Chem., Russia
Thermal Eng., Russia
Thermo. Fluid Dyn. (now *Heat Mass Transfer*)
Thermochim. Acta
Top. Appl. Phys.
Top. Curr. Chem.
Top. Curr. Phys.
Top Phys. Chem. Ser.
Top. Sulfur Chem. (A. Senning, ed.), (ceased publ.)
TRAC Trends Anal. Chem.
Trace Analysis (J.F. Lawrence, ed.)
Trans. Jpn. Soc. Aeronaut. Space Sci.
*Ukrainian Chem. J. (*formerly *Sov. Progress in Chem.*)
Vib. Spectra Struct. (J.R. Durig, ed.)
Vibrational Spectrosc. (Part of *Anal. Chim. Acta*)
Warme und Stoffubertragung (see *Heat Mass Transfer*)
World Energy Conference
Z. Angew. Math. Mech.
Z. Angew. Math. Phys., ZAMP
Z. Anorg. Allgem. Chem.
Z. Chem. (ceased publ.)
ZFW, Zeit. Flugwissen. Weltraum. (J. Flight Phys. Space Res.)
Z. Naturforsch. A. J. Phys. Sci.
Z. Naturforsch. B. J. Chem. Sci.
Z. Phys. D Atoms, Molecules, Clusters
Z. Phys. Chem. (Munchen)
Z. Phys. Chem. (Leipzig), (now merged with Munchen edition)

CHANGES TO THE JOURNAL/SERIES MASTERLIST

Advanced Materials
Advances in Atomic Spectroscopy
Advances Carbene Chemistry
Adv. Electron. Electron Phys. (now *Adv. Imaging Electron Phys.*)
Adv. Imaging Electron Phys. (formerly *Adv. Electron. Electron Phys.*)
Advances in Molecular Structure Research
Advances in Near Infrared Measurements
Advances in Theoretically Interesting Molecules
Applied Thermal Engineering
Astrophysics and Space Physics Reviews, Russia (formerly *Sov. Sci. Rev. E. Astrophys. Space Phys.*)
Bull. Soc. Chim. Belg. (now *European J. Inorg. Chem.*)
Bull. Soc. Chim. Fr. (now *European J. Inorg. Chem.*)
Calphad (Computer Coupling of Phase Diagrams and Thermochemistry)
Cambridge Monographs in Atomic, Molecular, Chemical Physics
Chemical Analysis (Book Series)
Chem. Berichte (now *European J. Inorg. Chem.*)
Chem. Eng. Research Design
Chem. Vap. Deposition (Part of *Advanced Materials*)
Chemistry Review, Russia (formerly *Sov. Sci. Rev. B. Chem.*)
Combustion Theory and Modeling
Compt. Rendus Acad. Sci., Paris, Ser. II. Part c. Chimie
Corrosion
European J. Inorg. Chem.
European J. Mechanics B. Fluids
European J. Org. Chem.
European Phys. J.
Fuel Processing Technology
Fuel Sci. Technol. Int. (now *Petroleum Sci. Technol.*)
Gazz. Chim. Ital. (now *European J. Inorg. Chem.*)
IEEE Trans. Plasma Sci.
Indian J. Chem. Technology
Inorg. Chimica Acta
J. de Phys. (now *European Phys. J.*)
Liebigs Annale (now *European J. Org. Chem.*)
Materials Chemistry and Physics
National Thermal Spray Conf. Proc.
Petroleum Science Technology
Physics Reviews, Russia (formerly *Sov. Sci. Rev. A. Phys.*)
Plasma Sources Sci. Technol.
Recueil (now *European J. Inorg. Chem.*)
Reviews in Mathematics and Mathematical Physics, Russia (formerly *Sov. Sci. Rev. C. Math. Phys.*)
Sov. Sci. Rev. A. Phys. (now *Phys. Reviews, Russia*)
Sov. Sci. Rev. B. Chem. (now *Chem. Reviews, Russia*)
Sov. Sci. Rev. C. Math. Phys. (now *Reviews Math. Math. Phys., Russia*)
Sov. Sci. Rev. E. Astrophys. Space Phys. (now *Astrophys. Space Phys. Rev., Russia*)
Surface Sci.
Theoretical Chemistry Accounts (see *Theoret. Chim. Acta*)
Topics in Fluorescence Spectroscopy
Z. Physik (now *European Phys. J.*)